SANS Data Reduction Tutorial

11/00 Version

This tutorial guides you through the basic features of data reduction using IGOR Pro.

For a "hands-on" experience, you may download the set of Tutorial Data, or use your own data, although there are some specific references to the Tutorial set. To work through the tutorial on your own, you must already have IGOR Pro and the SANS Reduction procedures installed. Once installed, open a blank data reduction experiment "SANS_Reduction_v3d.pxt", or a similar version. In addition to this help file, all SANS panels include balloon help (Mac) or command-line help (PC) that describes the action of each button or field in a panel.

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SANS Overview

The SANS Data Reduction using IGOR Pro is an implementation of the VAX data reduction procedures in an easier to use, graphical interface. It is designed to work on Macintosh or PC, and works directly on raw binary data files as they were collected on the VAX. All Raw SANS data files and reduction software can be carried to your home institution.

Typical use...

• During your SANS experiment, after your data is collected on the VAX, it is mirrored to a central server, "Charlotte". If your SANS account is NG3SANS41, your data will be located in the "NG3SANS41" folder on Charlotte. Charlotte is visible to Macs through Appleshare

(connect as a guest), and to Windows through the Network Neighborhood (NCNR group, Map the "SANS Data" folder as a network drive).
• With IGOR running on your computer (in the building...), you can work directly with the data on Charlotte. The data on the VAX remains untouched, as a backup. You can see and reduce the data while at the instrument, in the computer room, or in the user offices.
• Once your experiment is finished, all of your data - raw data files, averaged data, IGOR Demo version, SANS Reduction Macros... can be copied from Charlotte onto a Zip disk and carried home (a typical SANS session will produce between 2-6 MB of raw data). Data reduction can be completed (if necessary) at your home institution, without having to work around the NIST Firewall. FTP'ing of raw binary data from the NCNR to your home institution is not recommended, as the binary data structure is not always preserved, even in a "binary" transfer.
• Output of the data reduction procedures are ASCII files that can readily be read into your favorite graphics program.
• These ASCII files are also compatible with a collection of models that can be fitted to your SANS data. These models are available at:
<http://www.ncnr.nist.gov/programs/sans/igor2.html> , and use IGOR Pro's curve fitting features.

As of 11/2000, SANS Reduction macros were written using IGOR Pro v. 3.14. Future versions of the macros MAY use features only found in IGOR Pro v. 4.x. As always, the macros will work with free Demo versions of IGOR.

SANS System Requirements

• Macintosh or PC

• IGOR Pro installed <http://www.WaveMetrics.com> (v. 4.0 is the current version).
NOTE: You DO NOT need to purchase IGOR Pro to reduce your data. You can use either the (free) Demo version of IGOR Pro, or the full version. IGOR 3.1x or higher is required.
(The use of certain trade names or commercial products does not imply any endorsement of a particular product, nor does it imply that the named product is necessarily the best product for the stated purpose.)

• SANS Reduction Macros and the Tutorial data are available on our website:
<http://www.ncnr.nist.gov/programs/sans/igor1.html>
Follow the instructions on the webpage for downloading and installing the SANS Reduction Macros. Note that there are instructions for a (one-time) bug update if using IGOR 3.1x on a PC.

Instructions for the Impatient

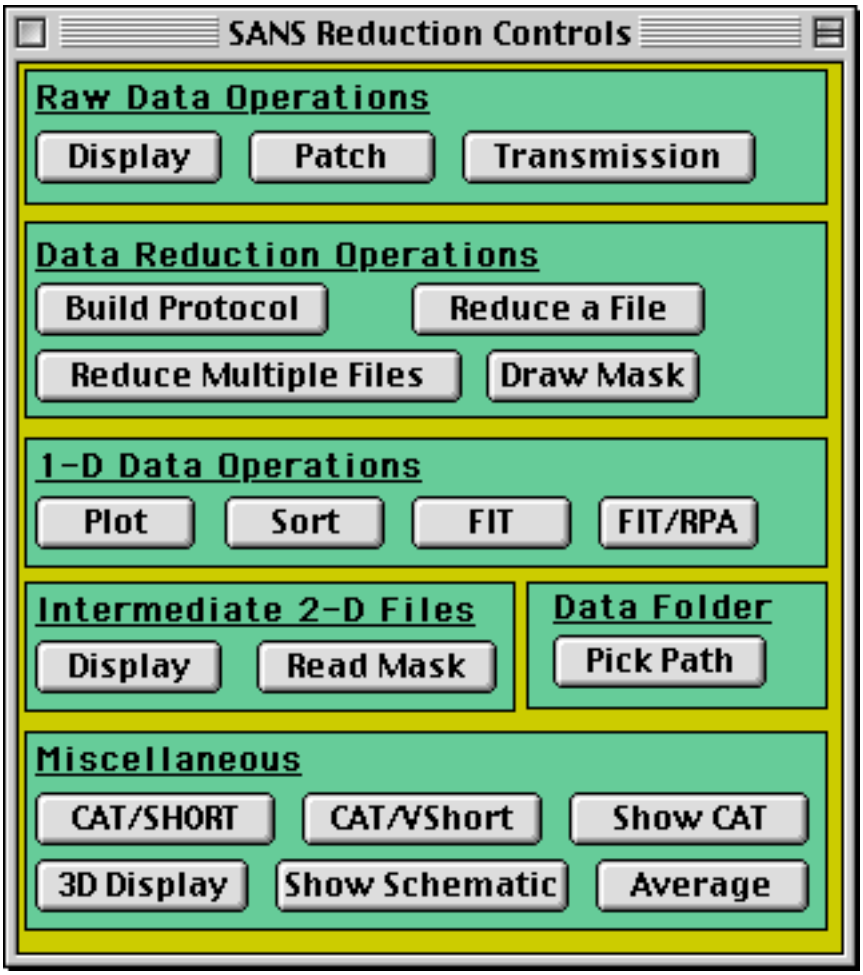
0) Open the "SANS_Reduction..." experiment
1) Pick the data path
2) List the data using CAT/VShort
3) Calculate transmissions
3) Build protocol(s) using CAT/VShort listing
4) Reduce files
5) Sort/combine the data
6) Write journal article

Main Controls

Why: To have the essential controls for SANS data reduction in one location.

What: Upon opening a blank template experiment for SANS data reduction, this main control panel is the starting point for viewing your data, performing the data reduction, plotting the averaged data, and performing some simple analysis.

How: The SANS Reduction macros are loaded and compiled upon opening the "SANS_Reduction..." experiment (this may take a minute or so on slower machines). After successfully compiling, the Main Panel of SANS Reduction Controls is automatically created. If you've lost this panel on the screen, selecting SANS->Initialize from the main menu bar will bring this window to the front. Clutter can be minimized by closing auxiliary panels when not in use. Panels are automaticallty re-created on demand.



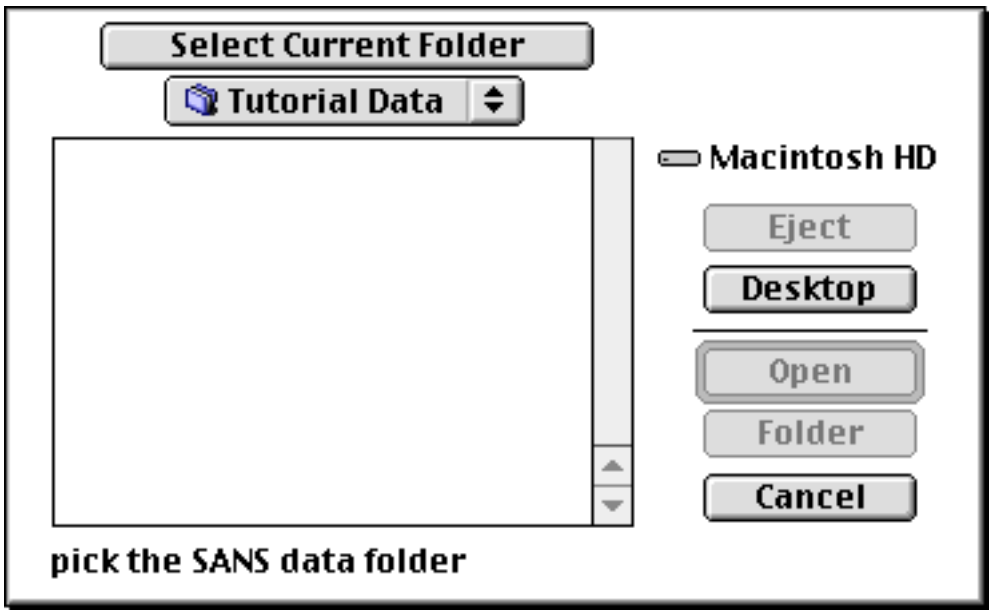
Listing the Data Files

Why: To see a table of your data files and associated information, and to have this table available for use in building reduction protocols.

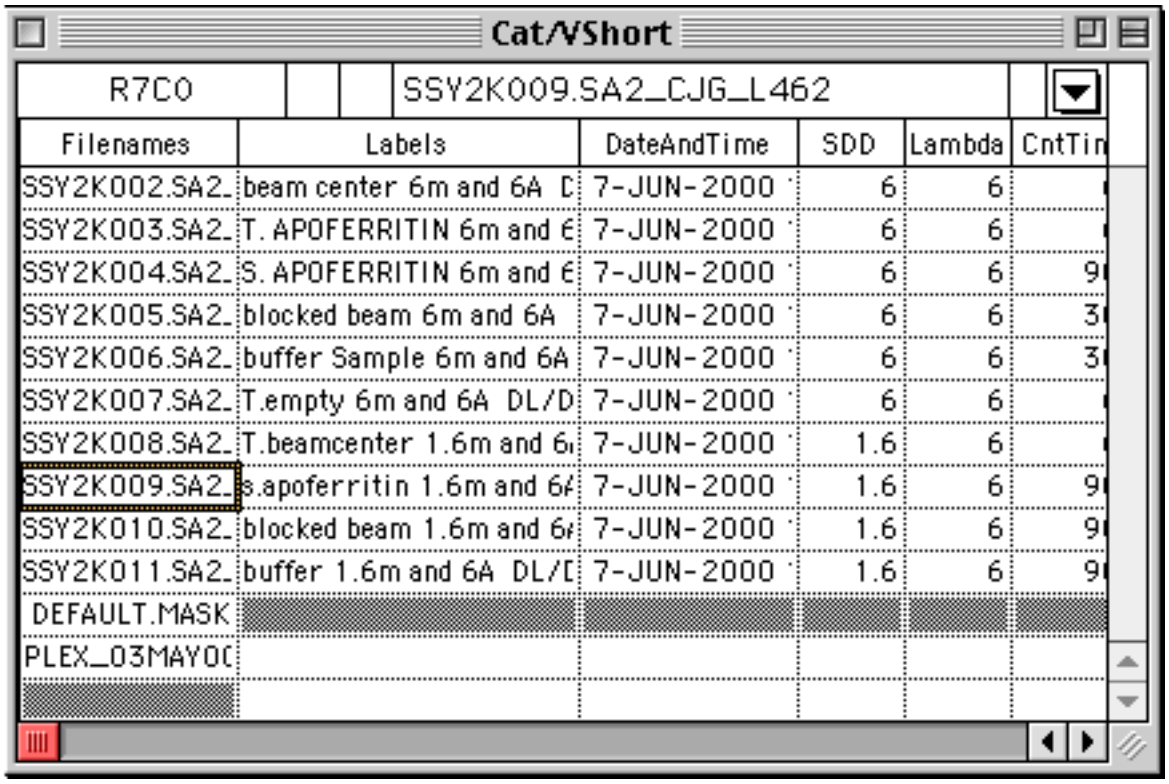
What: Set a path to your data folder, on Charlotte, then create a "Catalog" table

How: All of the raw data files, detector sensitivity files, mask files, etc. must be kept in a single folder for IGOR to access them. From the main panel, click "Pick Path" to set the path

to this folder. On a Mac, if your data is inside "Tutorial Folder", the dialog should look like this. On Windows it will look slightly different.



Now click "CAT/VShort" to create a catalog listing of all of the files in the selected folder. Raw SANS data files will show descriptive header information like the label, counting times, and thickness and transmission. The columns can be resized to see the whole label, etc., or delete columns of information you don't want to see. This table is also used interactively for building data reduction protocols, and is detailed later. Clicking "CAT/VShort" again will rebuild the list of files, and should be done if files were added to the folder or to confirm that header information was updated correctly. The table will list all of the files in the data folder, displaying information about raw SANS data files only. Files that are not recognized as raw SANS data are appended to the bottom of the "Filenames" column. Note that in the "Filenames" column, there are two additional files listed - these are the mask and detector sensitivity files.



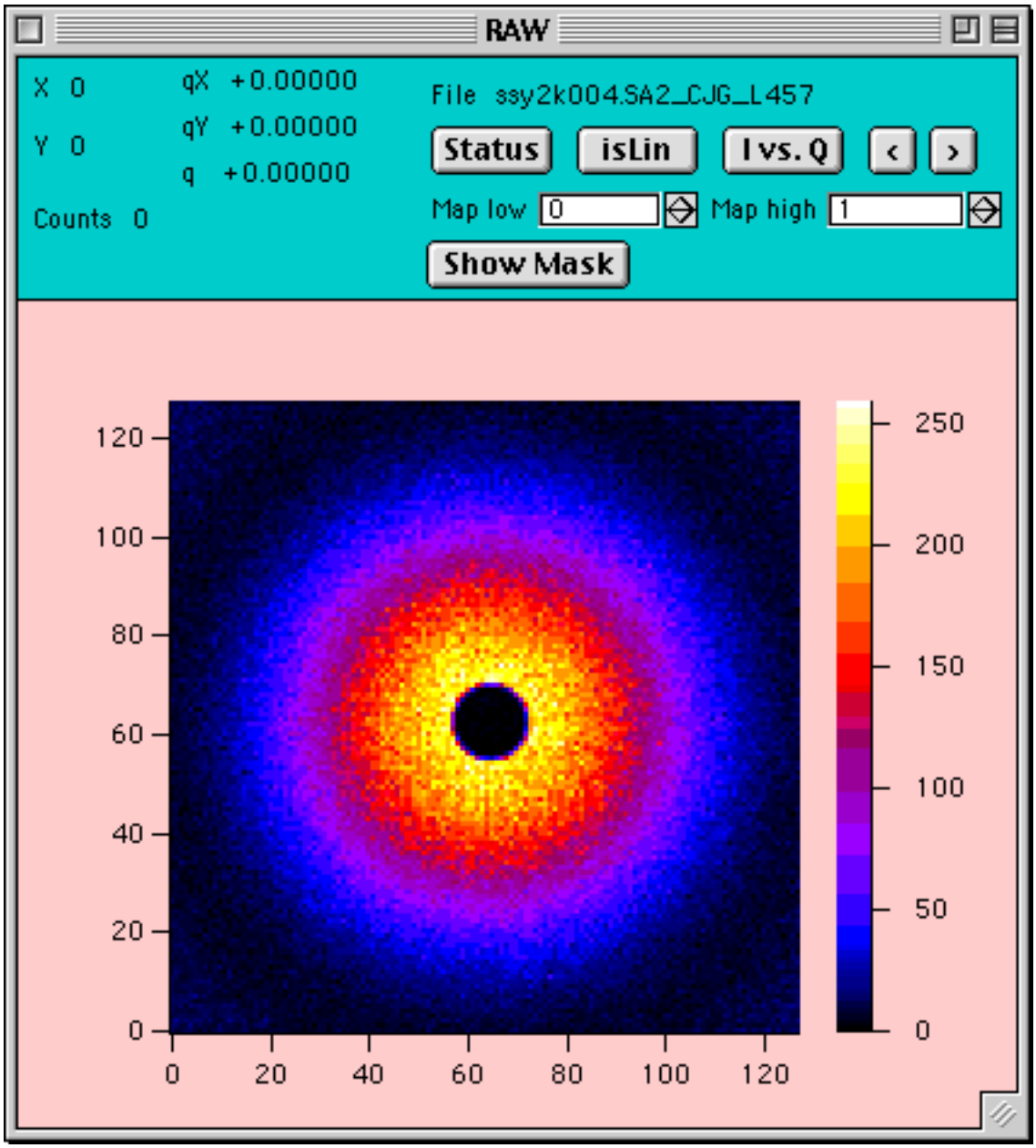
The Display Window

Why: To see what your raw 2-D data looks like.

What: Display a raw data file and get some simple information about the data

How: 2-D SANS data is displayed by clicking "Display" in the raw data operations box on the Main Panel. A standard dialog is presented to select the raw data file. The data is displayed, along with a scale bar. Important information about the data is displayed at the top of the graph, including the file, the (X, Y) position of the cursor, and the count value. If the display type is "RAW" then this is the actual neutron counts in that pixel. If the displayed data is one of the correction steps, it is no longer an integer neutron count value. The horizontal, vertical, and total q-value (in Angstroms^{-1}) is also displayed. Further information about the file can be displayed by clicking the "Status" button, and the information is displayed in the command window at the bottom of the screen. The count values of the data can be toggled between logarithmic and linear scale by clicking the "isLin" button. The current label on the button, either "isLog" or "isLin" gives the current scaling. The displayed data can be averaged (without doing any reduction steps) by clicking the "I vs. q" button. This will present a new panel with the Averaging Options. For averages of sectors or slices of the 2D dataset, the region to be averaged is marked on the dataset in response to the angles and widths chosen in the panel. The defaults are for a standard circular average of the full dataset.

If the data displayed is "RAW" data, and a path to the data has been chosen, left and right arrow buttons will also be present on the graph. This will display the next (or previous) run number in the data folder, if available, without having to proceed from the main panel though an open file dialog to select the file. The Map threshold values can be adjusted as desired to alter the color display of the data. The "Show Mask" button will toggle the currently loaded mask file (if present) on/off the dataset in a bright green color, indicating which data points are to be excluded from the 1-D average.



Averaging Options

Why: When doing an average over a selected region of the detector, it's best to see what is happening.

What: Open the Average Panel, and try out some different types of averages. The regions to be averaged are clearly shown on the data, and can be easily adjusted. The numerical vales of pixels, angles, etc. can be used in reduction protocols as well.

How: Open the Average Panel either using the "I vs Q" button on the Display window, or the "Average" button on the main panel. You wil then be able to average whatever data is currently in the display.

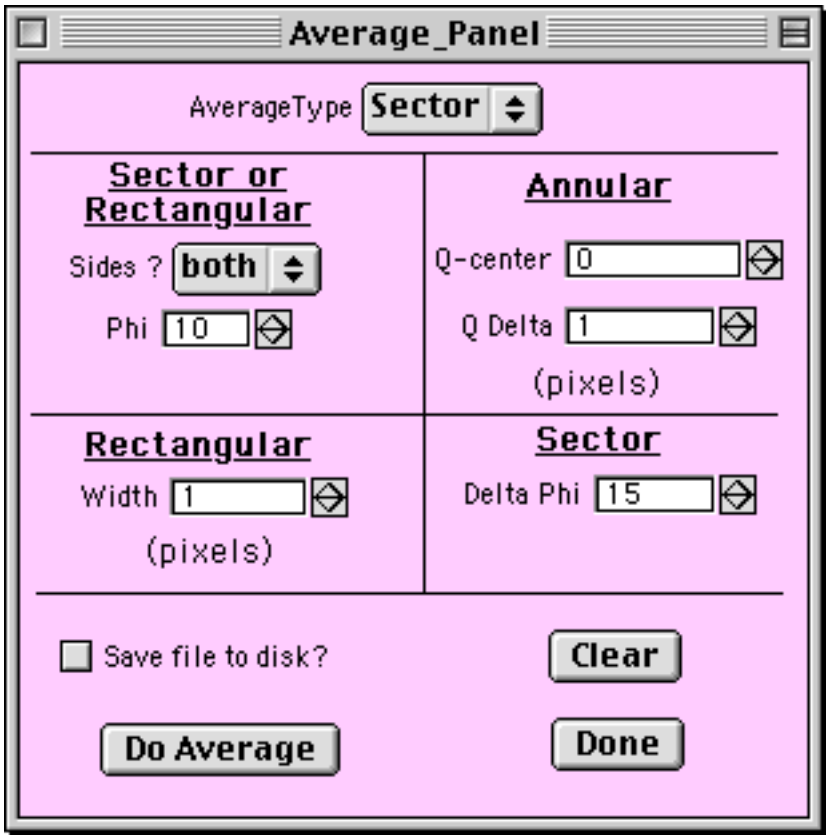
• "Circular" is the default average type. It will perform and average in constant q-rings around the (x,y) pixel location of the beam center. The default pixel width is fixed at one, and there are no other options to set when doing a circular average.

• "Rectangular" will average in constant q-arcs, but limited to a rectangular swath of a specified width of pixels. This rectangular swath can be oriented at any angle, and include either side or both sides of the detector.

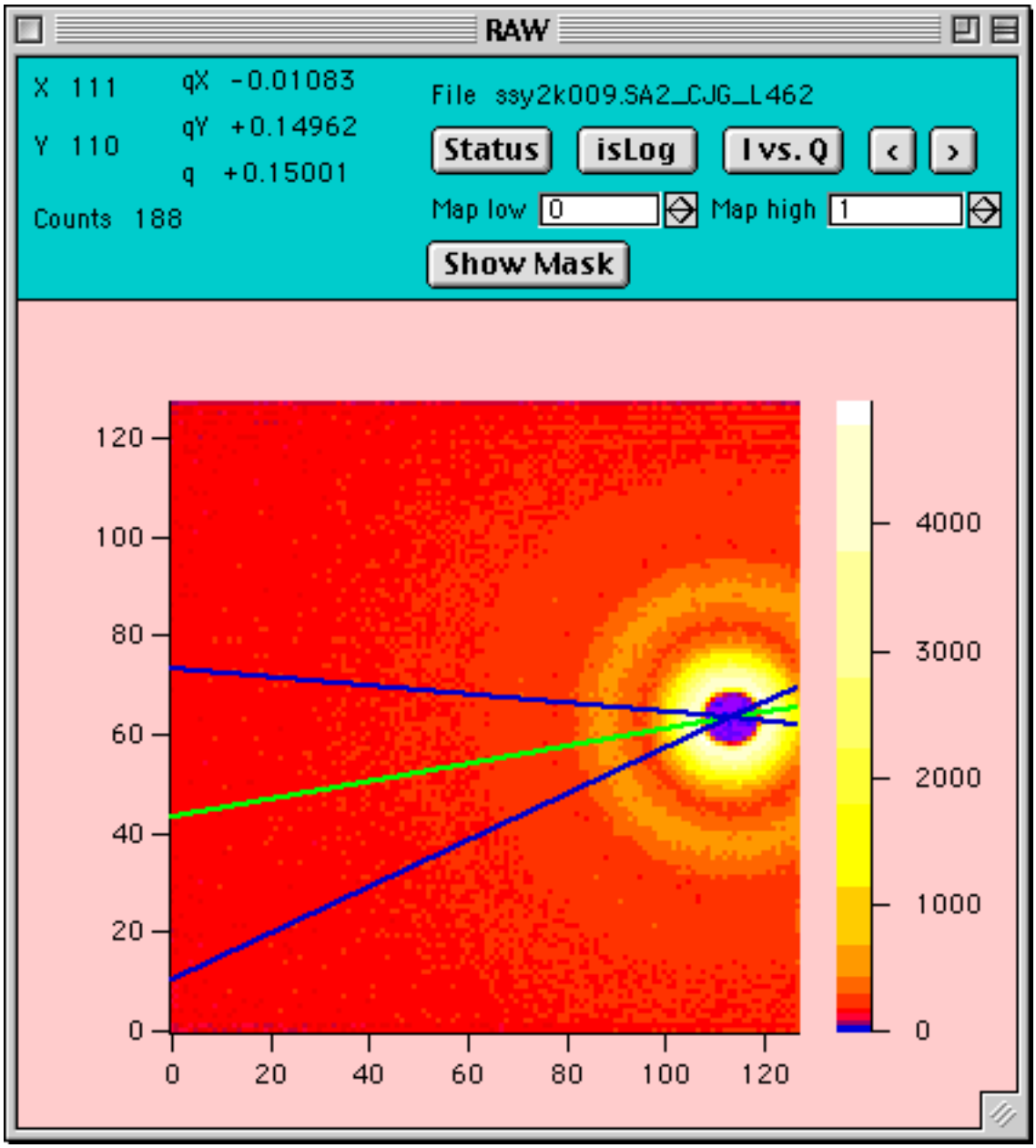
• "Sector" is very similar to Rectangular, except that the width of the sector is specified in degrees (+/- delta phi) each direction from the central angle (phi).

• "Annular" will perform an average centered at a single q-value (q-center), and averaged over a width of a specified number of pixels. The data is returned as a function of angle (phi) in degrees. If a normal x-y coordinate system is drawn through the beamcenter, zero angle corresponds to the positive x-axis and proceeds counter-clockwise. Therefore 270 degrees corresponds to the negative y-axis.

For this selection of sector average, and the angles phi and delta phi:



The corresponding Display shows what data will be included. The green line is the center of the average (phi) and the blue lines are maximum extent of the sector (+/- 15 deg = 30 degrees total angle).



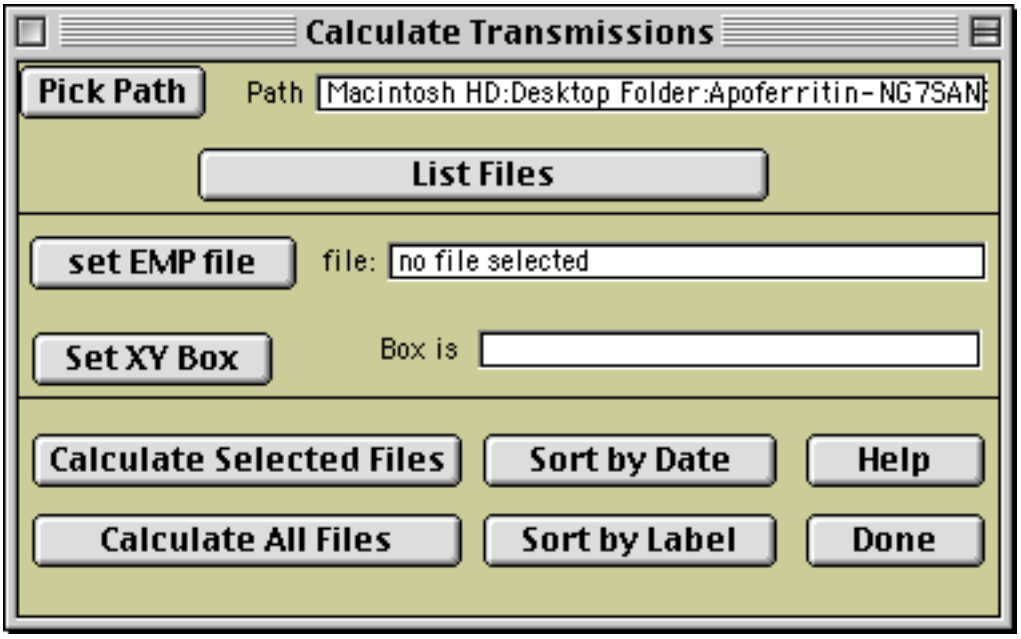
Averaged data that been saved from this panel (only if "Save File to disk?" is checked) will have "unknown" files listed as its protocol, since there's no way of knowing what steps have been performed on the 2-D data. If you know what you've done to the data, you're ok - it's just there as a warning.

Calculating Transmissions

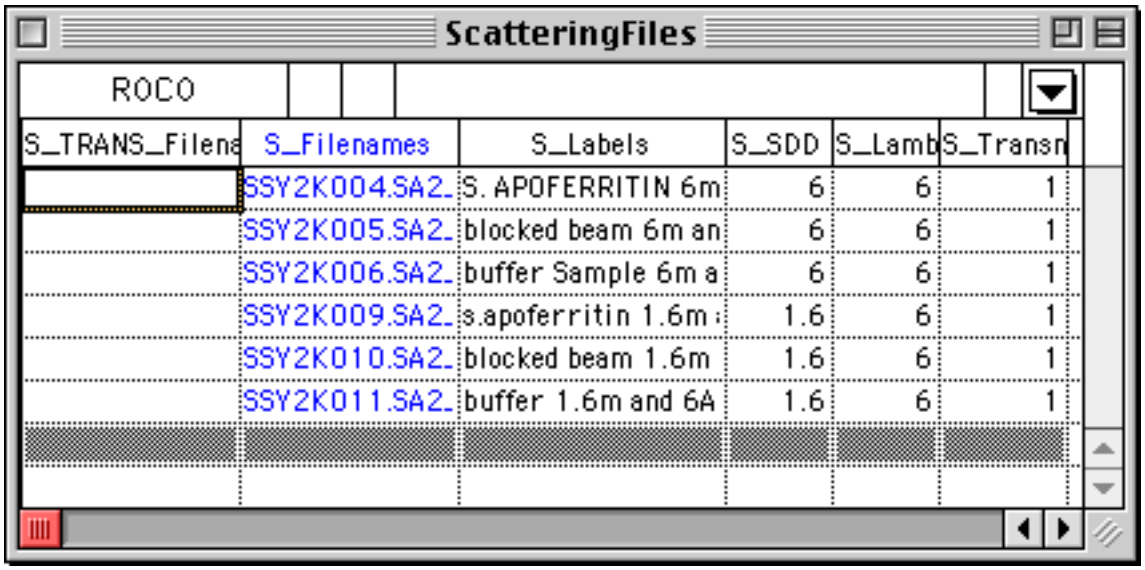
Why: Transmission of samples and sample containers must be calculated and entered into the headers of the raw data files for proper subtraction of non-sample scattering during data reduction.

What: Here we will create the "associations" between the transmission measurements and the scattering files to which they correspond. Transmissions will then be calculated and automatically patched to the file headers.

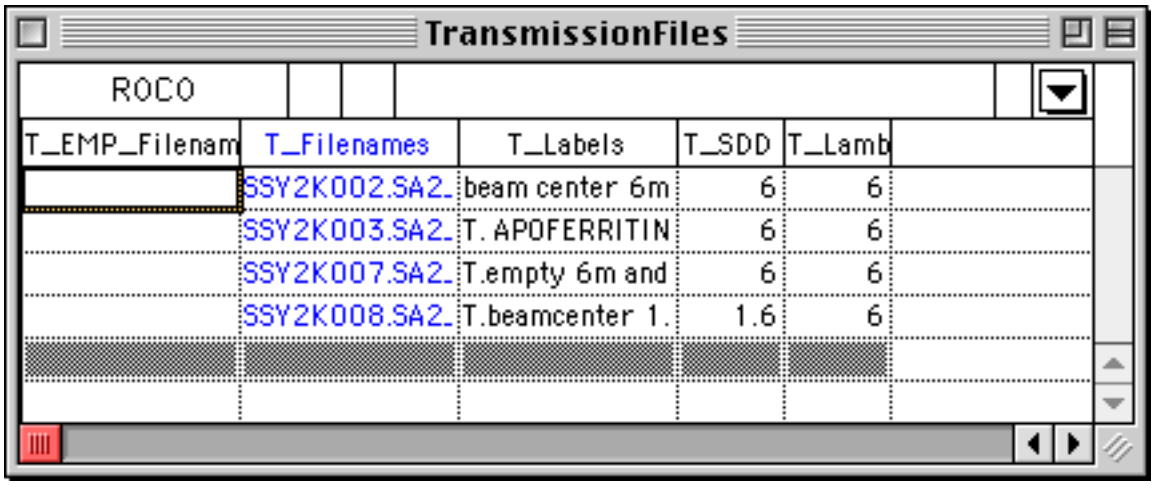
How: 1) Open the Transmission panel by clicking " Transmission" on the main panel. The following new panel will appear:



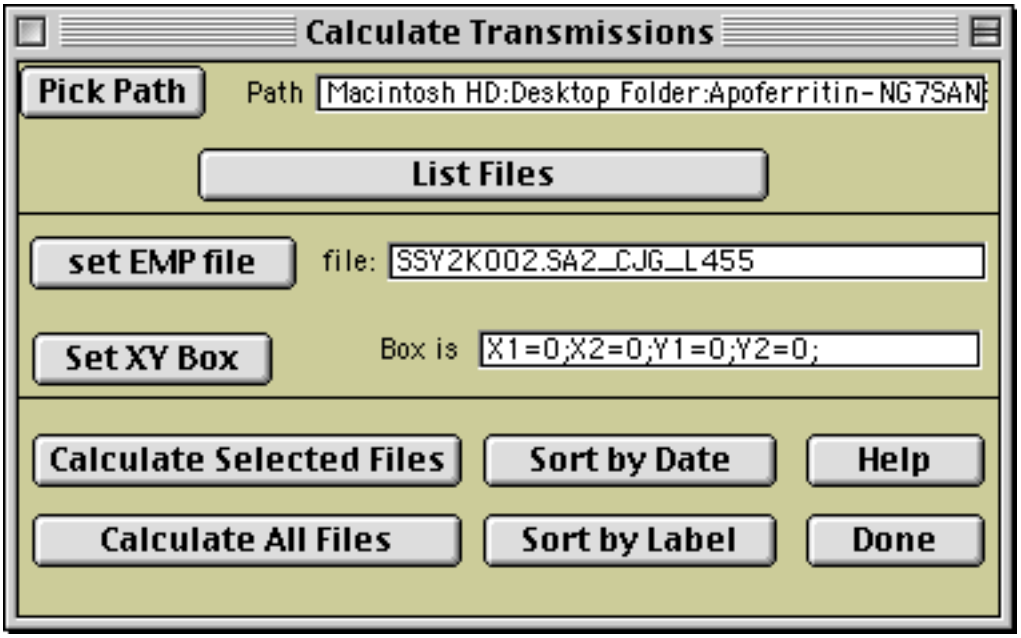
2) Click on "List Files" to build two tables - one with scattering files:



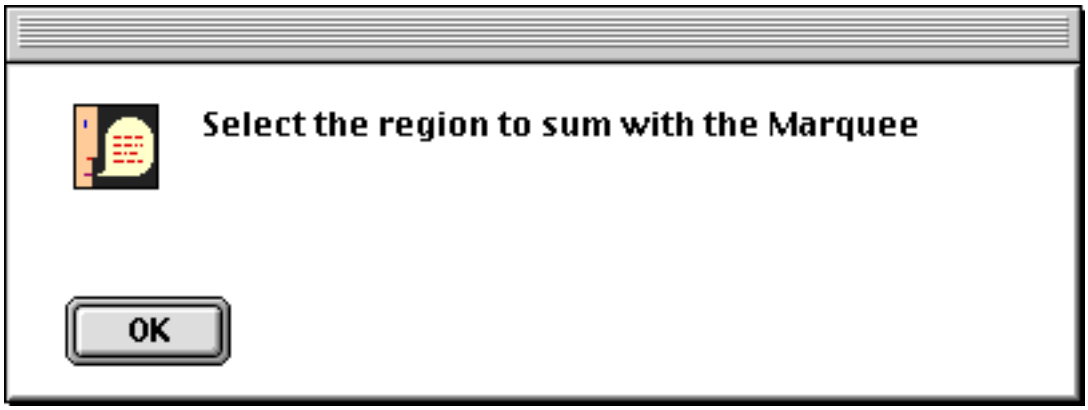
and another with transmission files. The transmission files are recognized from the file header by the beamstop being in an off-center position.



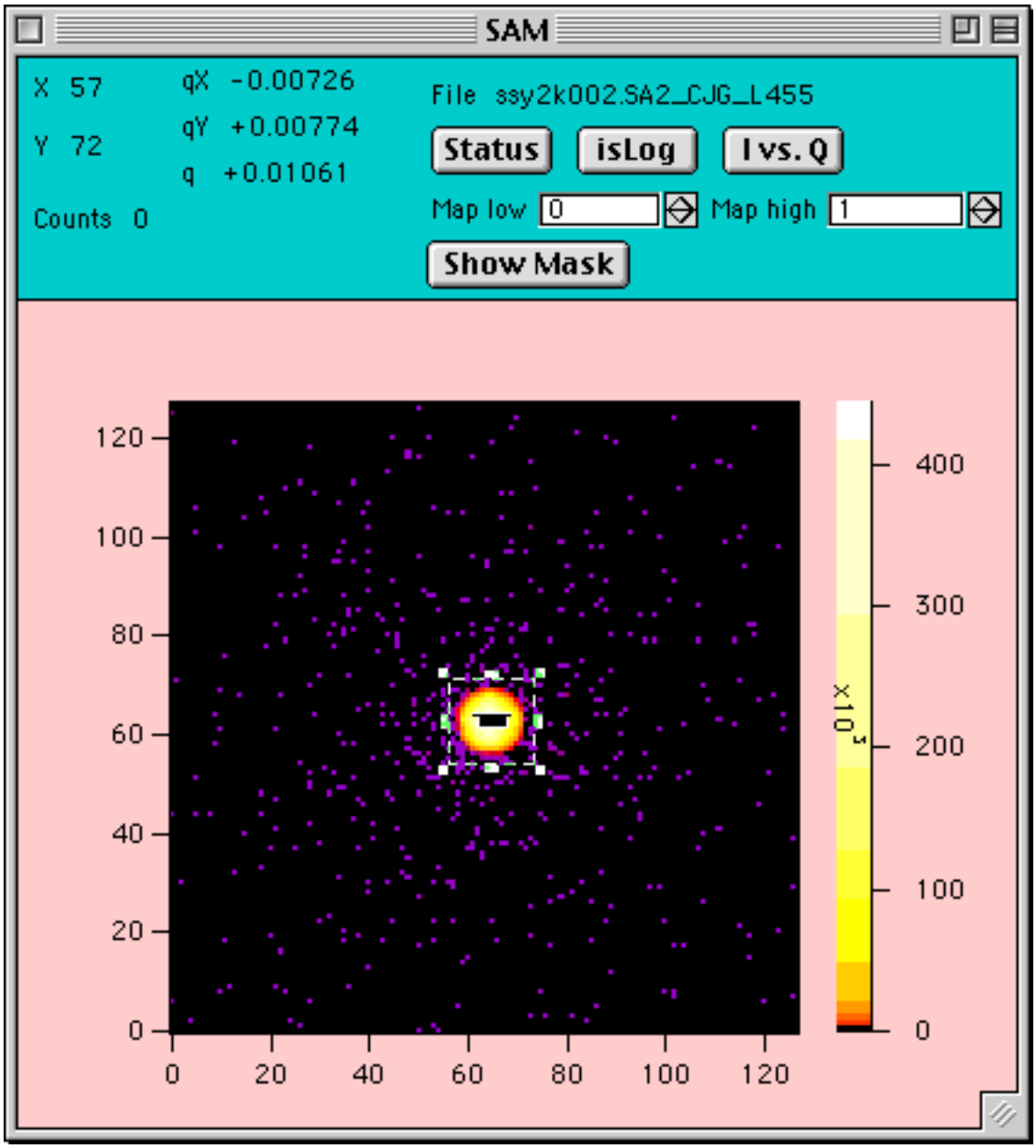
3) Find the empty beam transmission measurement in the TransmissionFiles table. It is in the blue "T_Filenames" column. For the tutorial, it is file SSY2K002.SA2..... Click on this file to select it (just that cell in the table). In the Transmission Panel, click "Set EMP File" to set this file as the empty beam. The filename appears, as well as the box coordinates:



The "intensity" of the empty beam is found by summing the number of counts on the detector over a specific rectangular region of the detector. Currently the box coordinates are zeros, so we need to pick the rectangle. Do this by clicking "Set XY Box". The raw data file (SSY2K002) will be displayed, and you will be presented with the following dialog:

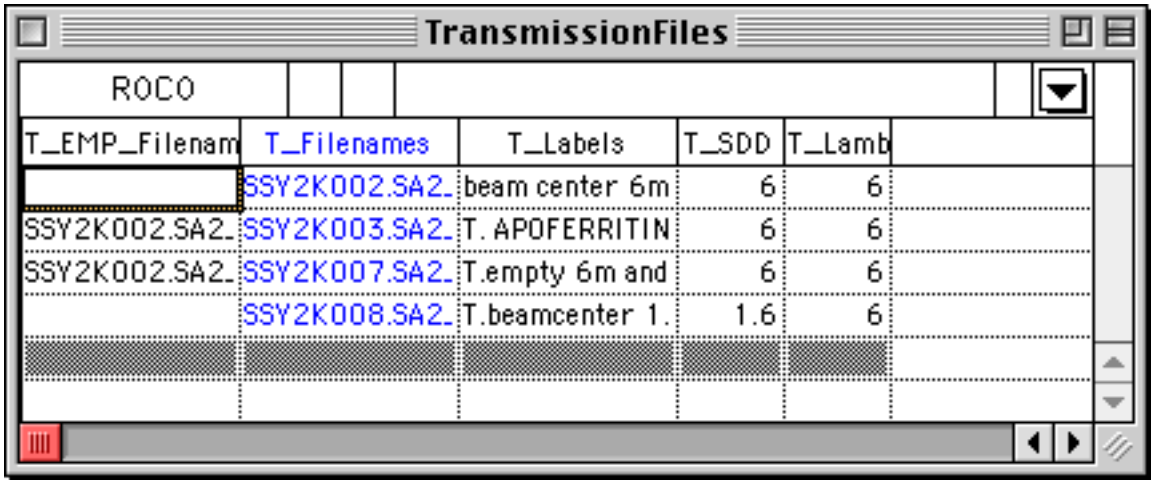


In the data display, click and drag a rectangle that encompasses the primary beam. You may find it easier to see the beam if you switch the display to log scale. Move the cursor inside the selection, to get an "upside-down hat" cursor.

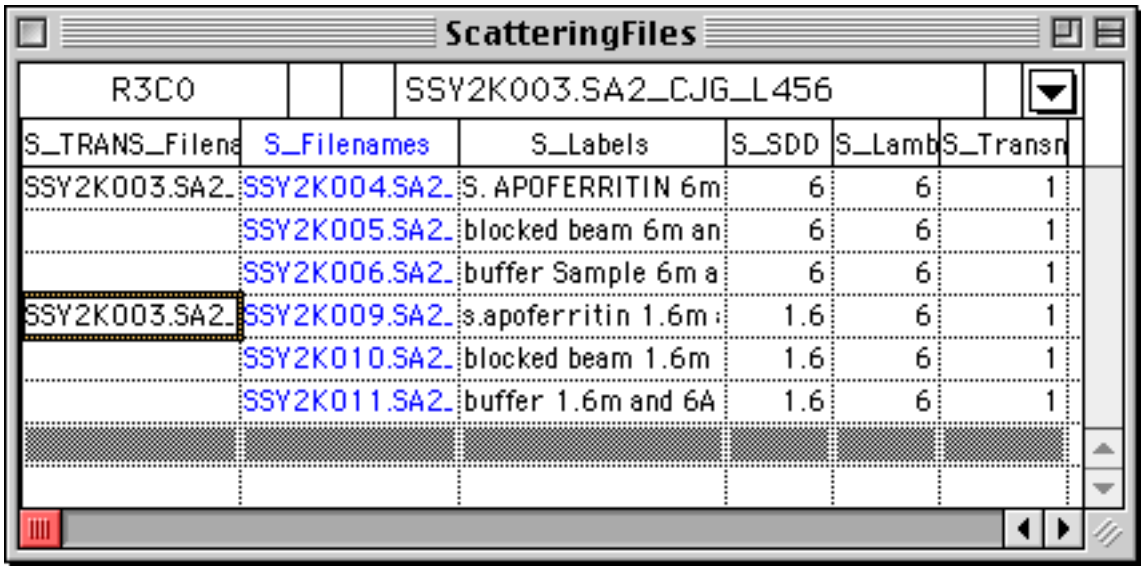


Click to get a menu, and near the bottom, select "Set XY Box Coords". The pixel values for the box should be updated to the Transmission panel, and are written to the empty beam file header for future calculations. You won't ever need to do this again. Note that the marquee selection can also be used to measure the beam center, or centroid of any selected region.

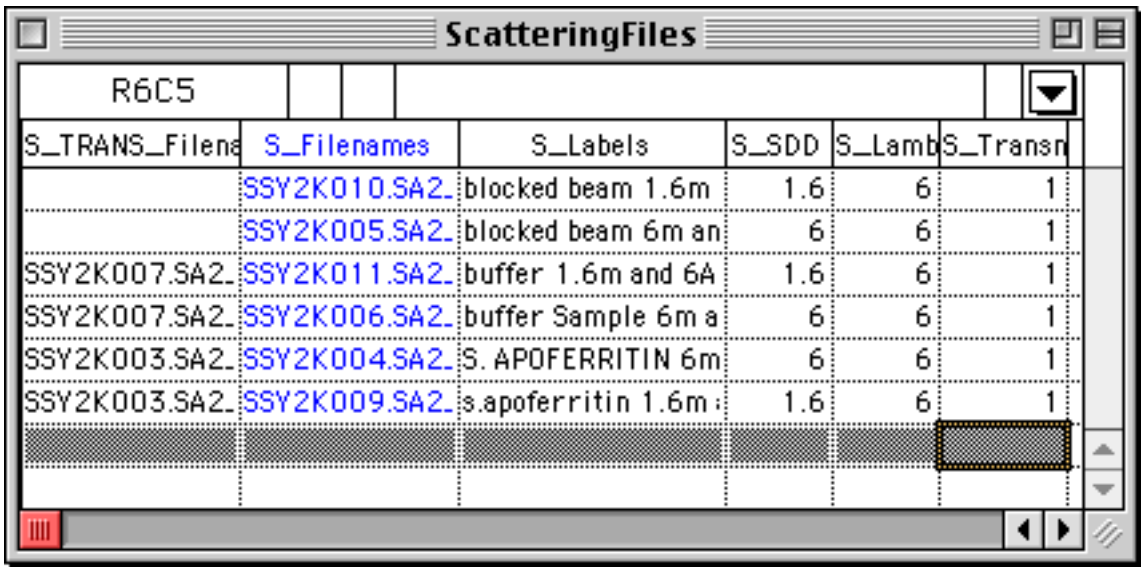
4) Now make the associations between the empty beam file and each of the transmission measurements. Each of the transmission counts will be normalized relative to the empty beam counts (and should therefore be less than unity). Make the EMPty beam association by selecting the empty beam file (in the blue column), copying it, and pasting the filename into the "T_EMP_Filename" column. You obviously don't need to associate the empty with itself, or with the beamcenter measurement that was taken at a different sample-to-detector distance (SDD). Transmission was only measured of two things: the apoferritin (a protein in an aqueous buffer, held in a quartz cell), and the buffer alone in the cell. Note that the sample label says "T. empty...", but it's really the buffer. You should try to do better with your sample labels. The TransmissionFiles Panel should look like this:



5) Now make the association between the transmission measurement of the apoferritin (SSY2K003) and the scattering file(s) for the same sample. In this case, the apoferritin scattering was measured twice - using two different instrument configurations. Copy the filename of the apoferritin transmission (SSY2K003...) from the blue "T_Filenames" column, and paste it into the (2) proper locations in the "S_TRANS_Filenames" column in the ScatteringFiles table, like this:

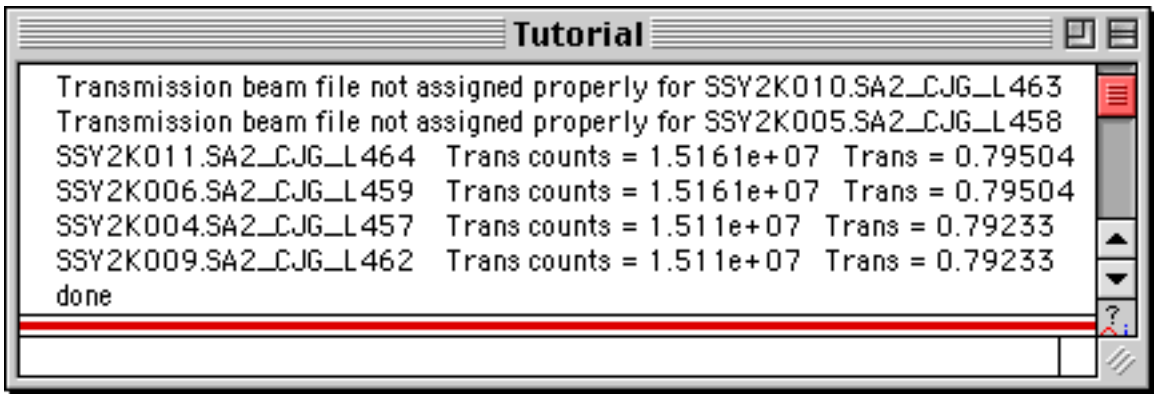


If you were consistent in your sample labels, it is often more convenient to group the same samples together, rather than a chronological listing of the scattering files. Click the "Sort by Label" button in the Transmission Panel to ge the following listing - note that the previous associations are carried along, and now the scattering measurements are conveniently grouped together. Do the same copy-paste (one at a time only) of the buffer transmission file (SSY2K007...) into the appropriate locations in the ScatteringFiles table. Note that there are no transmission files assigned for the blocked beam. We know that's zero, and the data reduction steps take care of that automatically. It doesn't matter if the file thinks that the tranmission is one (like it does currently). The ScatteringFiles table should look like this:



6) All of the proper associations have been made, so it's time to calculate the transmissions. "Calculate All Files" is the obvious choice from the Transmission Panel. The results of the calculation are displayed in the command window (usually at the bottom of the screen, cmd-J or ctrl-J will bring it to the front). The transmission files were not assigned properly for SSY2K010... and SSY2K005... which is not a problem, since these are our blocked beam files and we don't calculate the transmission of these files anyways. The other four files are calculated correctly, and these transmission values are automatically patched to the raw file

headers, and updated to the ScatteringFiles table. The CAT/VShort table, however, is not updated (unless you force it by clicking CAT/VShort on the main panel again).



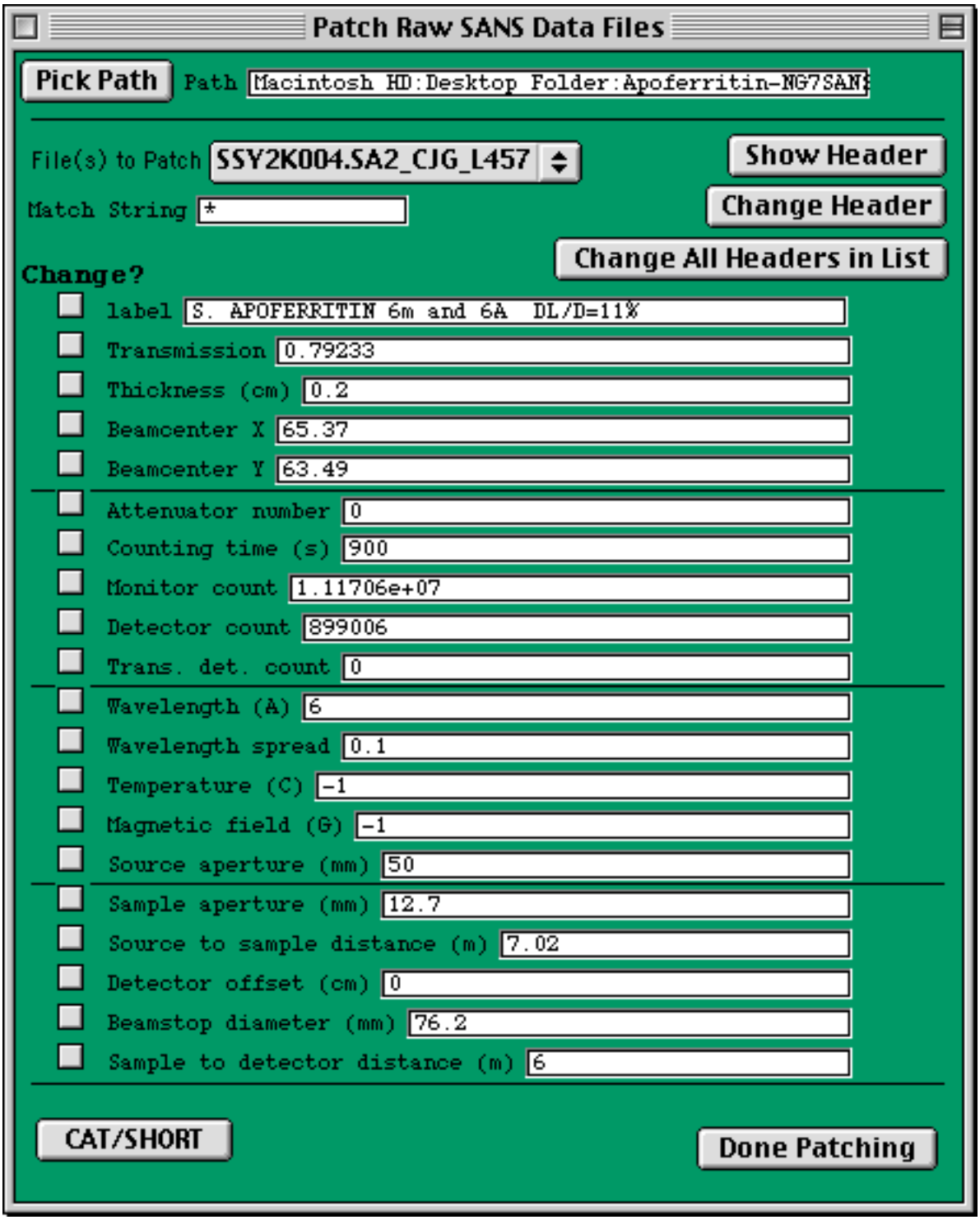
7) Transmission calculations are done. Clicking done will remove the panel and both tables. All of the tables and associations are regenerated by starting again from the "Transmission" button on the main panel. The previous associations are retained, and newly collected data files will have no associations. If the empty beam file had been previously set, it does not need to be set again, no matter what the panel indicates. Re-"setting" the EMPty file as in step 3 will show that the box coordinates are not zeros, but are the same coordinates that you previously selected with the marquee. In addition, if you only want to calculate the "new" files, select them in the blue "S_Filenames" column, and "Calculate Selected Files". It won't hurt to calculate all of the files, but it is a waste of time.

Patching File Headers

Why: Some of the information in the file header may have been incorrectly set at the time of data collection, and must be updated before data can be correctly reduced.

What: Actually change header values in the raw data files. Be sure you know what you're changing before you do. Typically, no information needs to be changed here, since transmissions were "patched" previously.

How: From the main panel, click "Patch". This will display a new panel that can be used to verify and change certain fields in the raw data headers. If the data path is not set, do it now using the "Pick Path" button. Click (and release) the popup menu of files to refresh the list. Since the Match String is "*", all data files will be shown. The "*" has the usual wild-card meaning. Only a single wildcard can be used to trim the list of files displayed in the popup. The header information in the displayed file in the popup is shown below it in the text fields. If, for example, you want to change the sample label, you simply enter the new text into the box, check the "change" box next to it, and click "change header". If the "change" box is not checked, that field cannot be changed in the file header. This feature prevents accidentally changing values you don't intend to change. To patch the same information to a series of data files (like the beam center X and Y) enter the new values and check the "change" boxes. You can use the match string to trim the file popup to include the files that you want to change (you may have to change the files in a few batches to change just the ones you want). Then click "change all headers in list". You will be warned that it will change more than just the top file, and say "yes" to change all the files in the list. Transmissions were calculated previously using the Transmission panel, and should all be correct here.



Building a Data Reduction Protocol

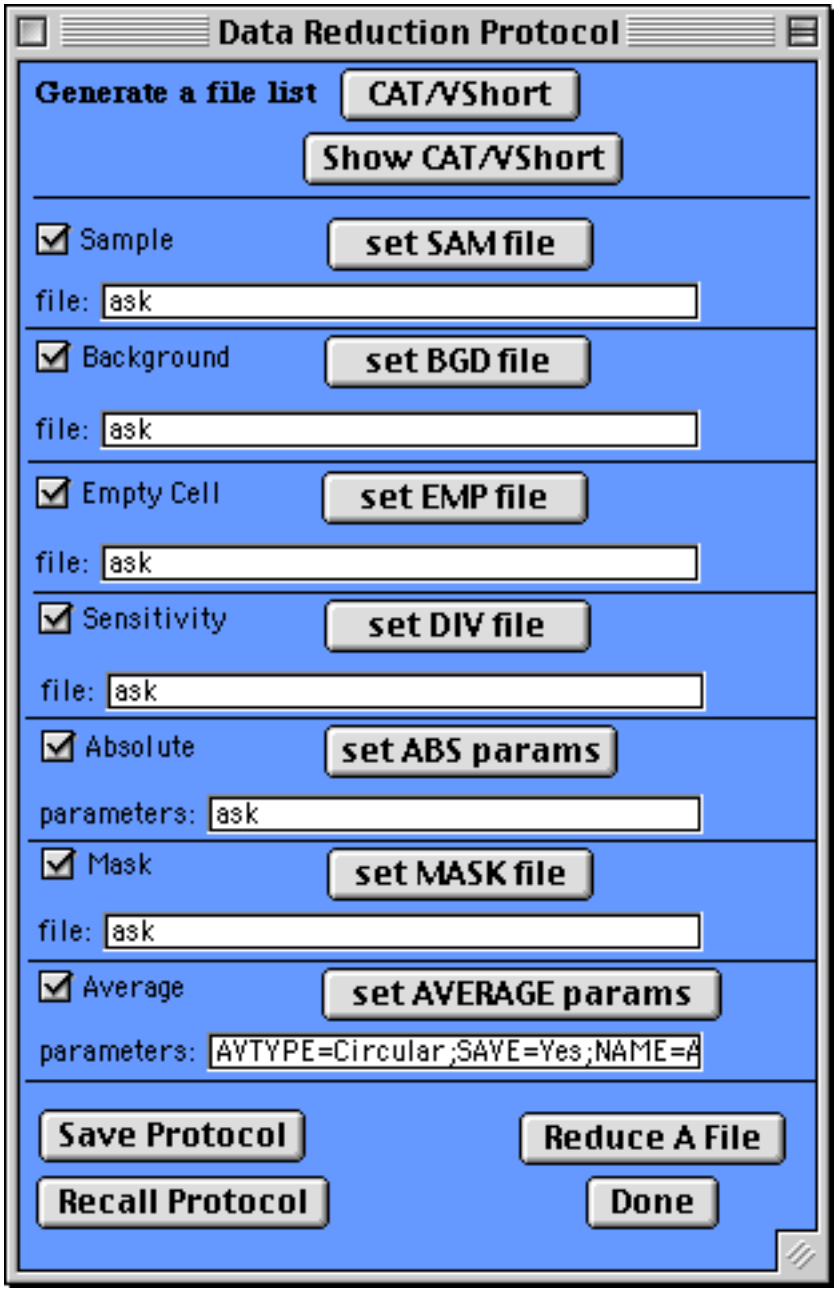
Why: Building and saving a protocol allows you to repeatedly reduce raw data files for a given configuration using the same exact sequence of corrections.

What: Identify the files and steps necessary to correct your data for non-sample scattering, detector sensitivity, convert to absolute scaling, eliminate "bad" detector pixels, and produce averaged 1-D ASCII output. Once a protocol is constructed for a specific instrument

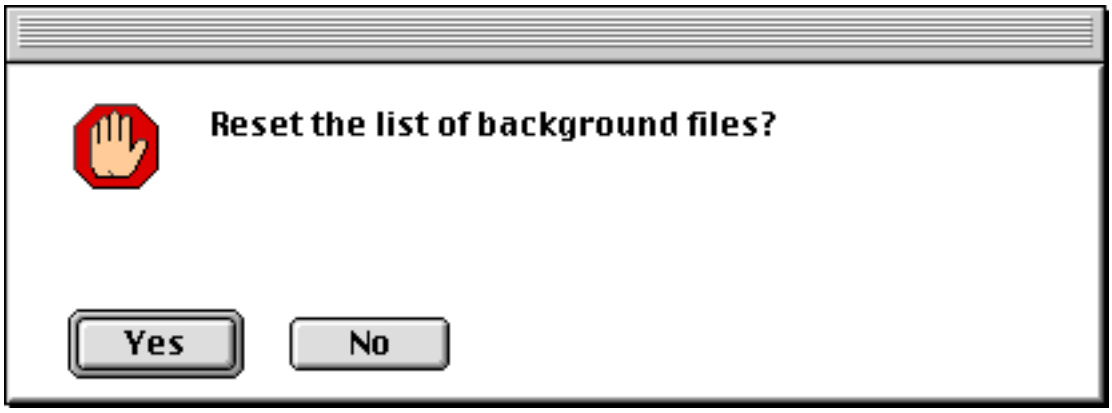
configuration, it can be saved and recalled for later use.

How: Click "Build Protocol" on the main panel. This will present a new panel with a list of reduction steps that can be used. Steps that are checked will be performed, steps that are not checked will be skipped (except that you will always supply a sample file, or be prompted for one). For this example, we will use all of the data reduction steps, and first build a protocol to reduce data taken at a 6 meter sample to detector configuration and use absolute scaling from an empty beam measurement. Click "Show CAT/VShort" to bring the listing of files to the top, and arrange the windows so the list and the panel are visible.

a) Leave the sample field as "ask" so that the program will prompt us for the sample data file(s) when they are needed. We could specify a file to bypass the dialog, if desired.



b) Fill in the background file by finding it in the listing (run SSY2K005), clicking to select the filename, and then clicking "Set BGD file" on the panel. The following dialog appears:

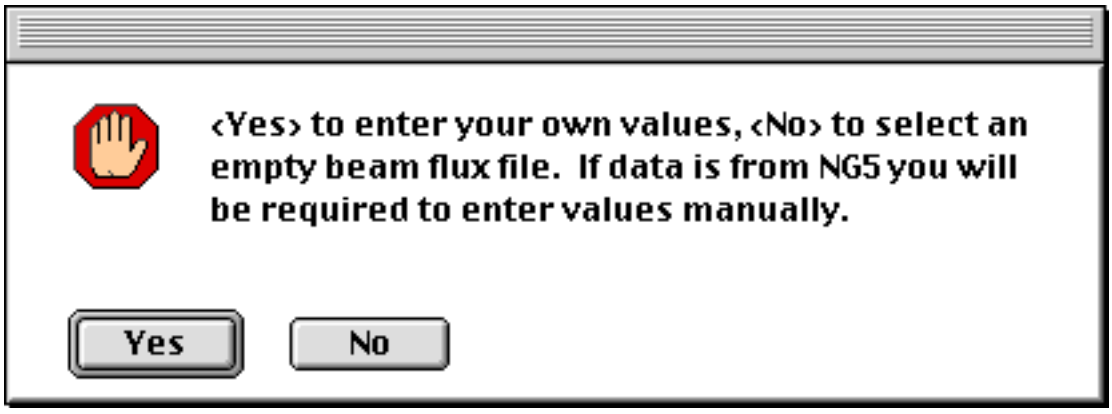


Say "Yes" to reset the list of files. This will set this single file (the selected text) as the background file. If several background files were collected and it is desired to add them together, reset the list for the first file, and then select "No" (don't reset) for additional files to add together. These additional files will be listed in the field as well and added together during the data reduction. The EMP (and SAM) file fields are set in an identical fashion.

c) Fill in the EMPty cell file (actually the buffer solution, in this example) in the same way that the BGD file was set. It is run SSY2K006.

d) Set the detector sensitivity (DIV) file. The file is PLEX_03MAY00_NG7.DIV (at the bottom of the CAT/VShort table). Note that it is not a raw SANS data file, and is not recognized as such by the listing. There can only be one detector sensitivity file assigned to a protocol.

e) Set the absolute scaling parameters. Click the "set ABS params" button, and the following dialog appears:

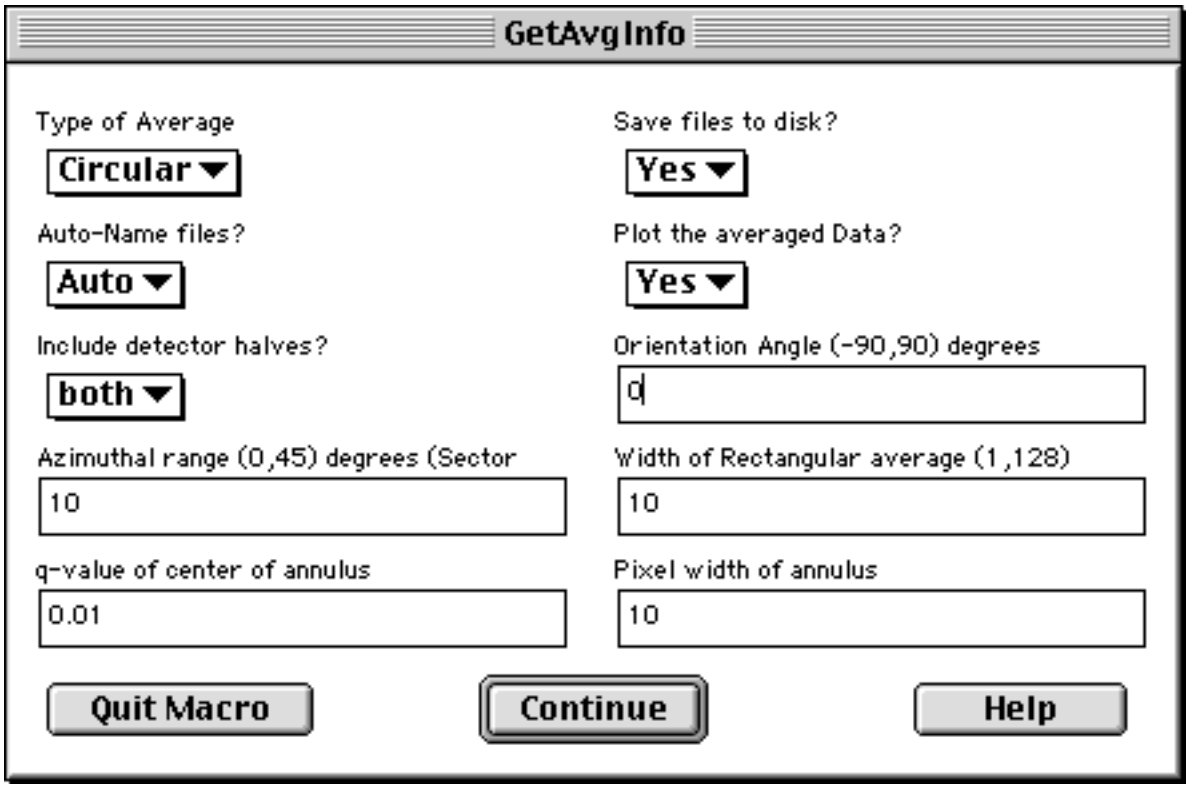


Select "No" and you will be prompted for an empty beam measurement (at 6 meters) to use for absolute intensity calibration. When the dialog appears, select run SSY2K002..., which is the empty beam measurement. The file will be opened, and the absolute scaling parameters will be calculated and listed in the field on the Protocol Panel. If you are using a measured secondary standard for calibration, "Yes" will allow you to enter your own values (i.e. the standard thickness, transmission, I(q=0), and the tabulated cross-section of the standard sample).

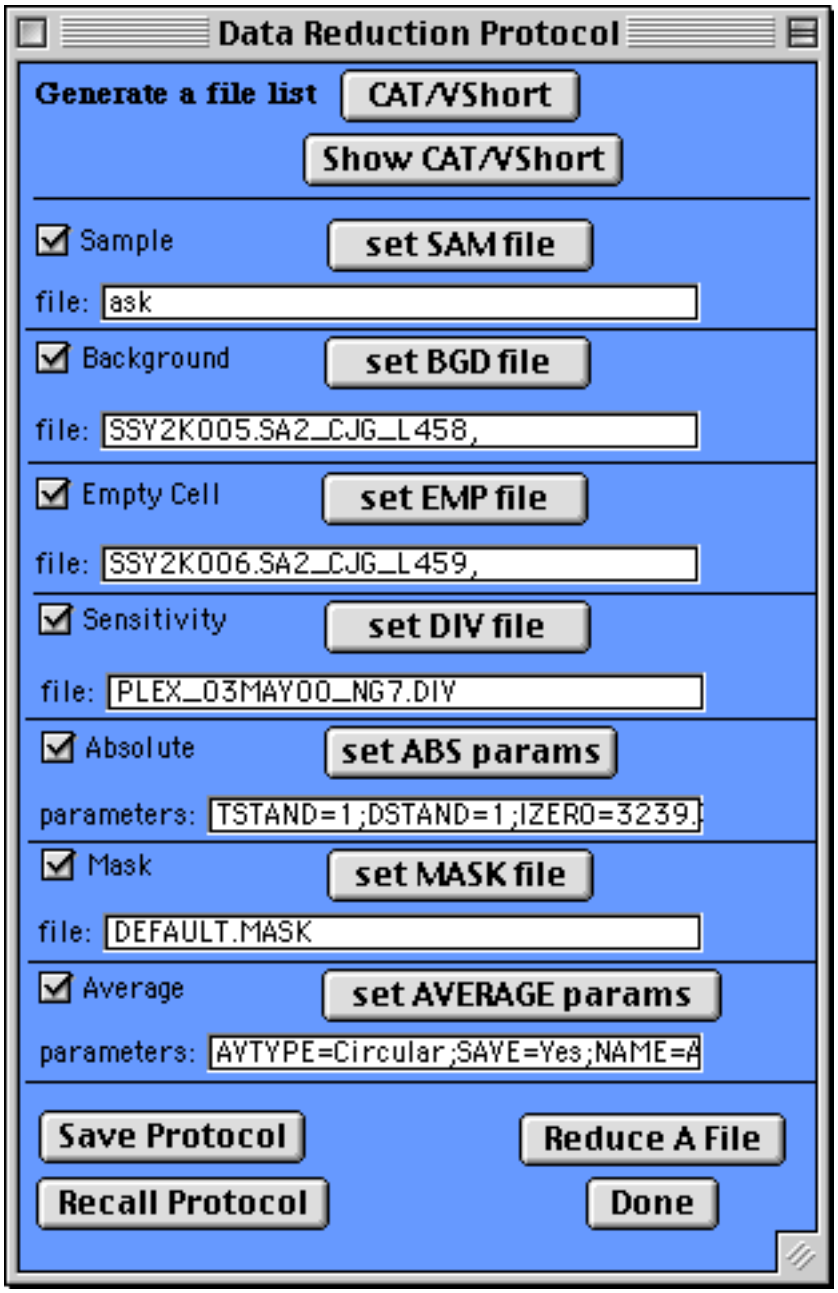
f) Click on the "DEFAULT.MASK" filename in the listing, which is a simple mask to exclude the edges of the detector. Click "set MASK" to set the filename. The mask file was created

either in IGOR Pro or in SANS Image. Note that this is NOT the same format as a "WORK.MSK" file from the VAX.

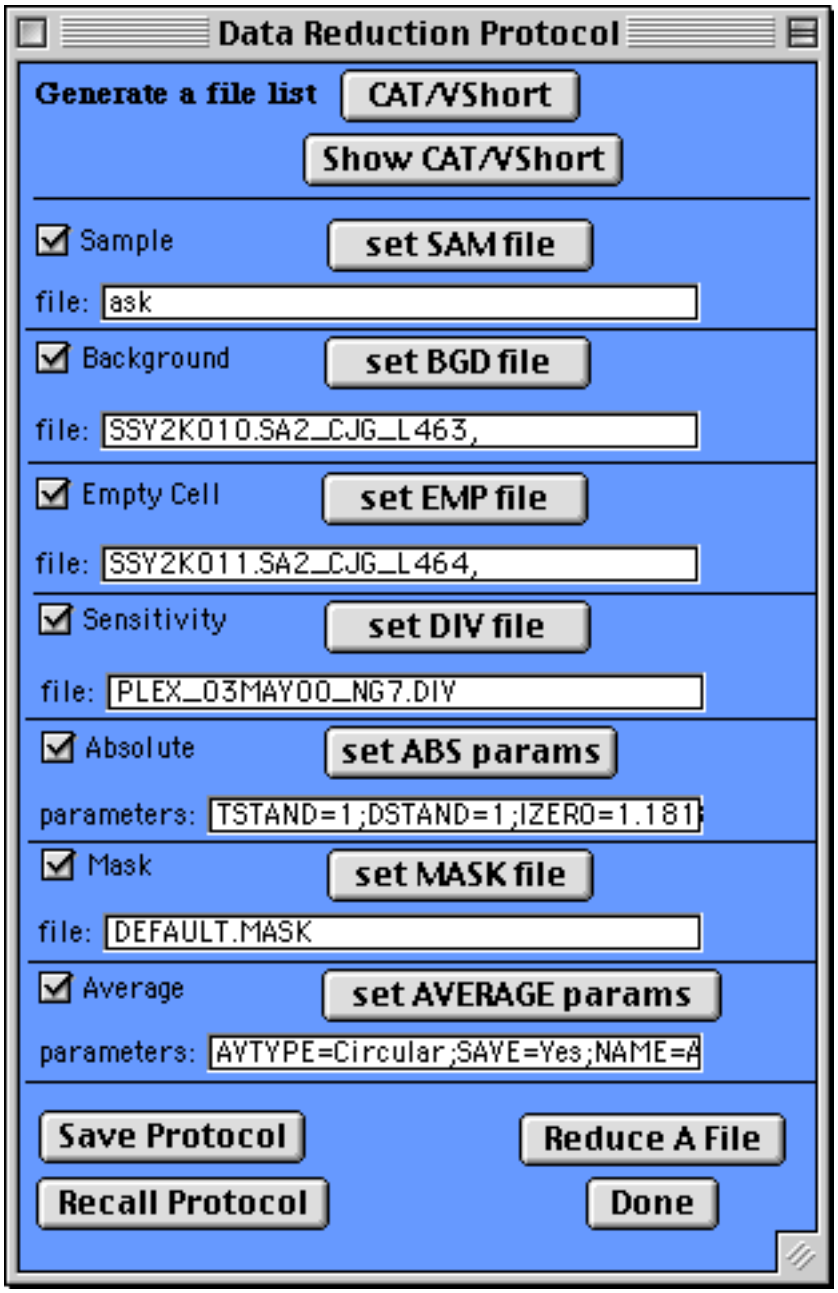
g) Default values for a circular average of the data (annulus width is always one pixel) should already be in the field. If not, or a different average is desired, click "set Average Params", and set the desired values in the dialog. Note that some of the fields do not apply for a given type of average, and their values are irrelevant.



h) Once all fields are set to their correct files / parameters, click "Save Protocol" to save these settings for later recall, using a descriptive name for the protocol. "sdd_6meters" is a good choice for this protocol. Your Protocol Panel should look like this:



i) Set up another protocol to reduce the data at the 1.6 meter configuration. This involves selecting a different background file, empty cell (buffer) file, and empty beam file for absolute scaling. The mask and detector sensitivity files do not need to be changed, nore do the averaging options. The Protocol Panel should now have the following information. Save this protocol as "sdd_1_6meters" or something else descriptive.



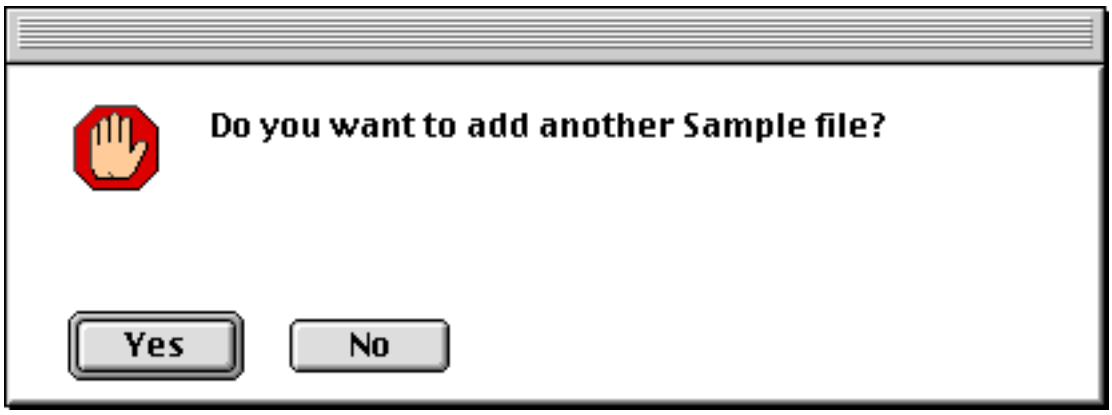
Reducing a File

Why: If I have to explain why...

What: Process a raw SANS data file to a 1-D average using a previously saved protocol, or use a blank protocol where you will be prompted for each data file as needed.

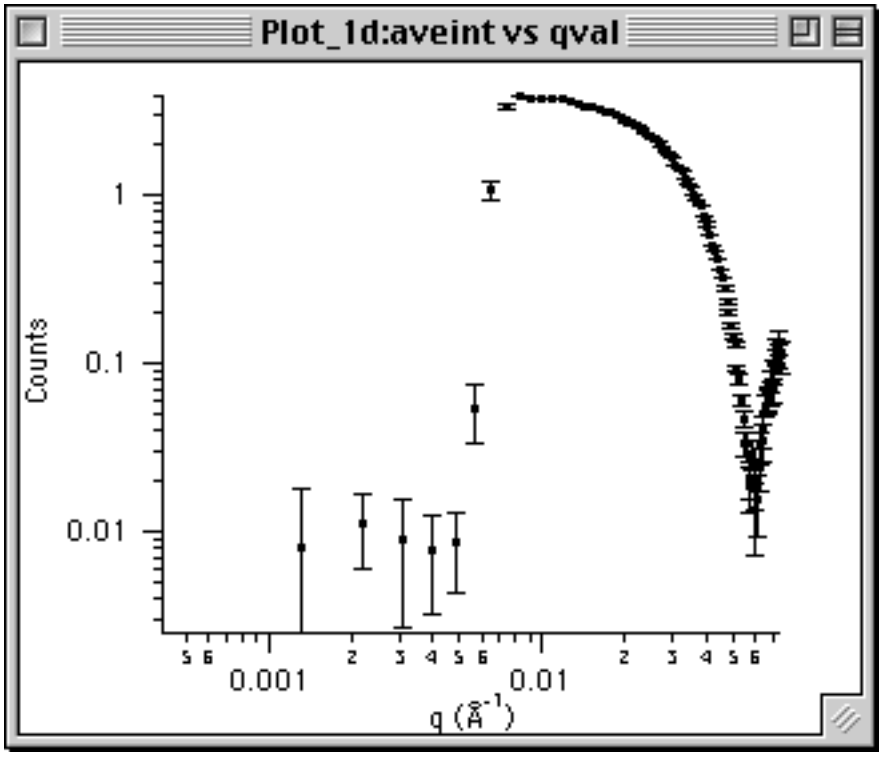
How: Since we just created and saved our two protocols, we'll use them directly from the Protocol Panel. Start with the 6-meter protocol. To make sure it's in place, click "Recall Protocol" on the panel, and pick "sdd_6meter", or whatever you named it from the list. Your protocol choices are updated in the panel. At this point, you can either choose the 6-meter apoferritin scattering file from the CAT/Short window, and "Set SAM File", or since the protocol says "ask", just let it prompt you with a file dialog. Either way, click "Reduce A File" on the Protocol Panel. Pick the scattering file from the dialog if prompted (it's run

SSY2K004...). The file wil be displayed, and you will be prompted to add another sample file, if desired:



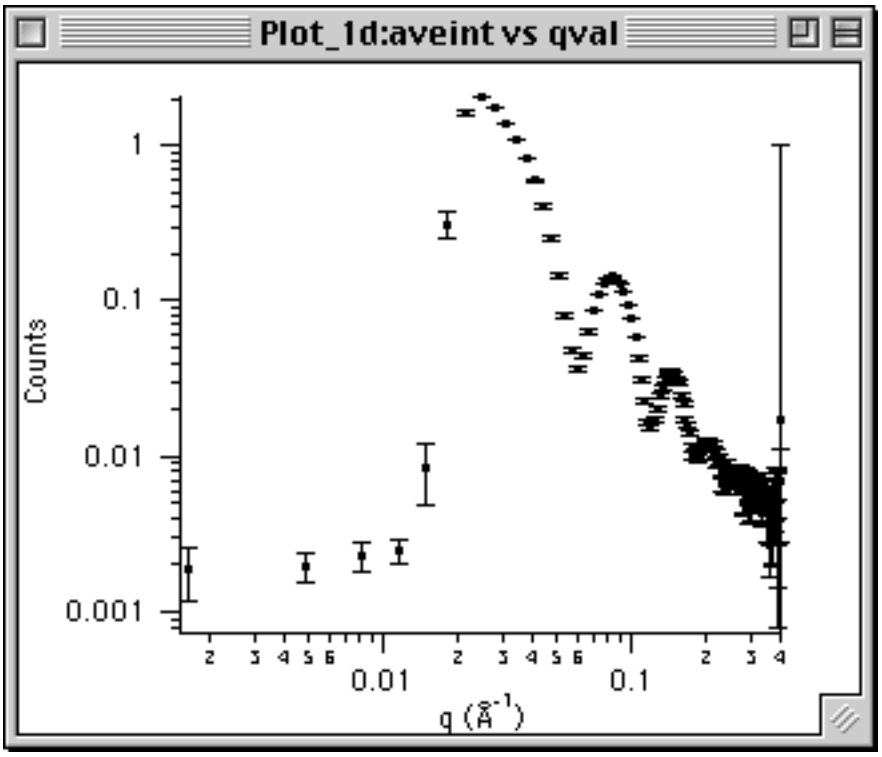
If you re-measure a sample at the identical configuration, you can add these raw data files together to improve the counting statistics. In this case, we only have one file, so (No) we don't want to add another data file.

The data reduction wil proceed through the protocol, showing each intermediate step along the way. Watch closely - if something doesn't look right, go back and check it out after the reduction is done. If something is grossly in error, the reduction can be aborted (cmd-. on Macintosh, or the Abort button at the lower left in Windows. This example will proceed smoothly, of course. The final result should look like this, and the command window should indicate that a data file was written, and what filename was used.



• For the second data file, we'll use another method to reduce the file. Close the Protocol Panel, and click "Reduce A File" on the main panel. From the popup, choose the protocol for the 1.6 meter configuration "sdd_1_6meter" (or whatever you named it) and click continue.

You will be prompted for the sample scattering file (it's SSY2K009...) and the reduction will complete as before, using the files specified in the protocol. The final result for the high q data should look like this:



Instead of building a protocol, one could use either the "Base" protocol - which does only minimal corrections, or "DoAll" which will perform all of the data reduction steps. To see exactly which steps each of these would perform, "Recall" these blank protocols into the Protocol Panel. Unchecked steps in the protocol will be skipped, and "ask" will prompt you to pick the required files from a standard dialog.

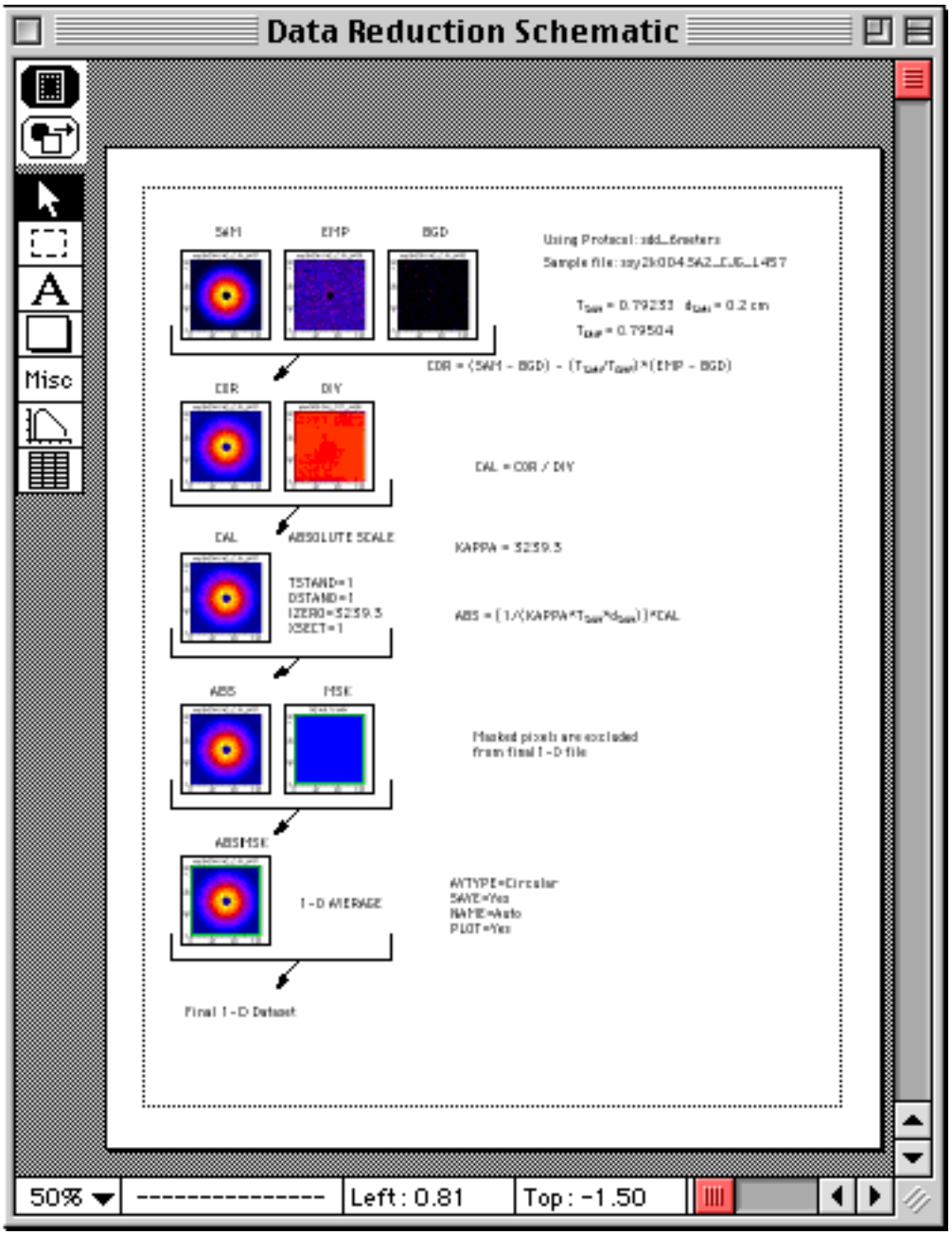
Schematic of Data Reduction Operation

Why: To see what happened at each step of the way during the data reduction. Very useful for diagnosing problems in data reduction. NOTE: if you are using a demo version of IGOR Pro, you will not be able to do this step (sorry), but you will be able to view the intermediate files individually, by using the Miscellaneous Operations.

What: Reduces a data file using a previously saved protocol, and creates a printable layout showing all the details.

How: To see what steps were used and what the files looked like, click "Show Schematic" on the main panel. When prompted for the protocol, choose one that you just created and saved. You will then be prompted for a "Sample Data file" - choose the appropriate scattering run again, and it will be reduced again in exactly the same way. Once the reduction is complete, small images of the intermediate steps will be created, and placed in a layout window. This can be inspected (or printed in color) to see exactly what data files were used at each step, what numerical constants were used and what file was saved. A placeholder box titled "Not Used" is in place of steps that were not used (at your request) in the reduction protocol. A placeholder box titled "No Data" means that you wanted to use that step, but an error occurred, and no data could be found (usually a file has been improperly

specified).



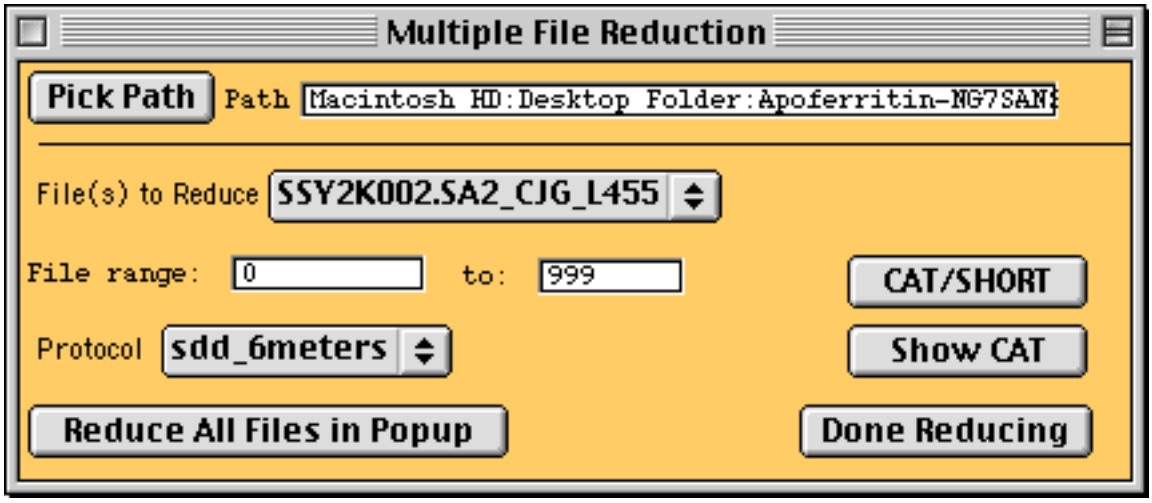
Reducing Multiple Files

Why: Reducing a block of files collected at the same configuration is faster than reducing them one-at-a-time.

What: Consecutively numbered runs at a given instrument configuration (corresponding to a constructed protocol) can be reduced in a batch mode. The data files MUST be consecutive - otherwise a protocol will be applied, with unhappy results, to raw data files from a different instrument configuration. Even with this restriction, data can often be reduced in blocks of 7-10 files.

How: Since this tutorial only works with one file at each instrument configuration, no

data will be processed here. Click "Reduce Multiple Files" on the Main Panel. This will display a new panel with a simple interface. By setting a range of run numbers (leading zeros are not needed) this range of raw data files will be displayed in the popup list. Select the appropriate protocol from the popup (you must have already created / tested / saved it from the Protocol Panel) to be used to reduce the selected files. Click "Reduce All in Popup" to reduce all of the files in the list with the chosen protocol. All the intermediate steps are shown, for each file reduced. Automatic naming is the best choice in a protocol when reducing multiple files, since no input is required from the user.



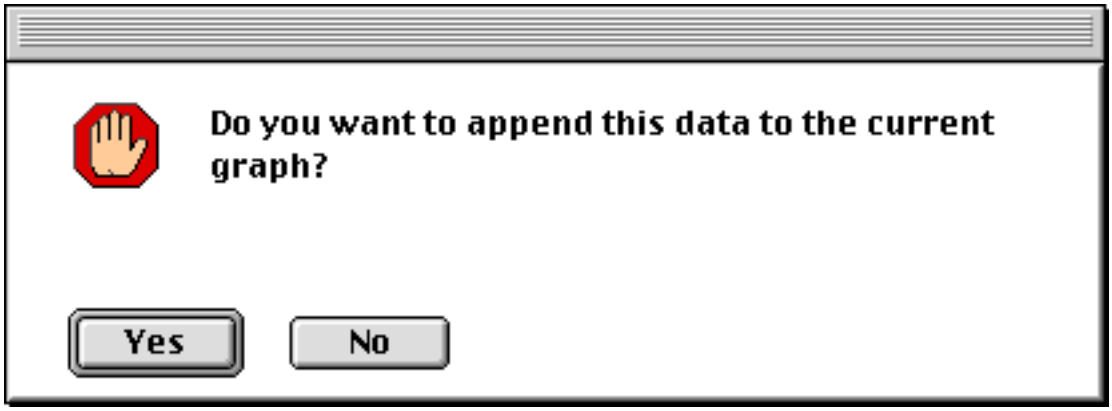
Plotting Averaged Data

Why: To see one or many averaged data files.

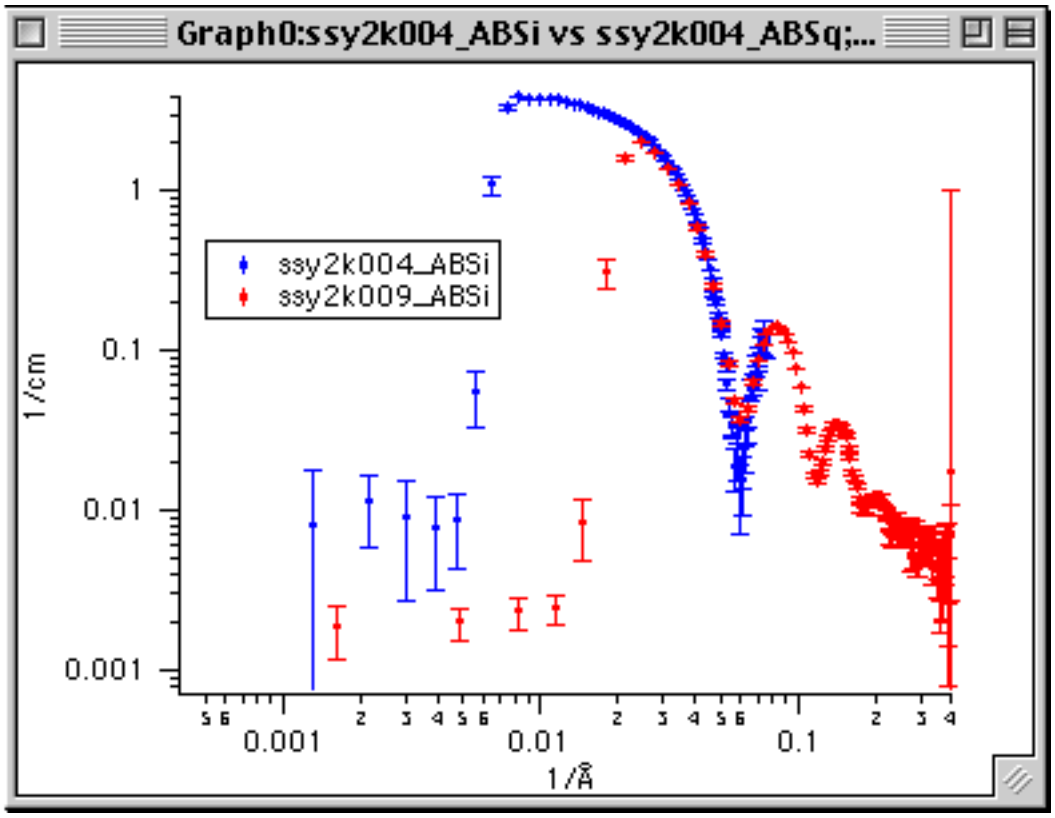
What: Plot 1-D averaged data on a log-log scale (default) and plot multiple datasets on the same graph.

How: Click "Plot" on the main panel, and a dialog will be presented for you to select the file to load. If the file has not already been loaded, it will load and automatically be graphed. To change the graph appearance, click on what you want to change, and a dialog will appear. The Graph menu also allows customization of graphs.

• If the top window is a graph, you will be presented with the option to add the data to the "top" graph:



PLOTting both of the apoferritin files (either order) will generate a graph like this:



NOTE: The 2-D Display window is also a graph. If the Display window is on top, you don't want to overlay a 1-D dataset on top. If you do, the display will look garbled - just close the display and it will redisplay correctly.

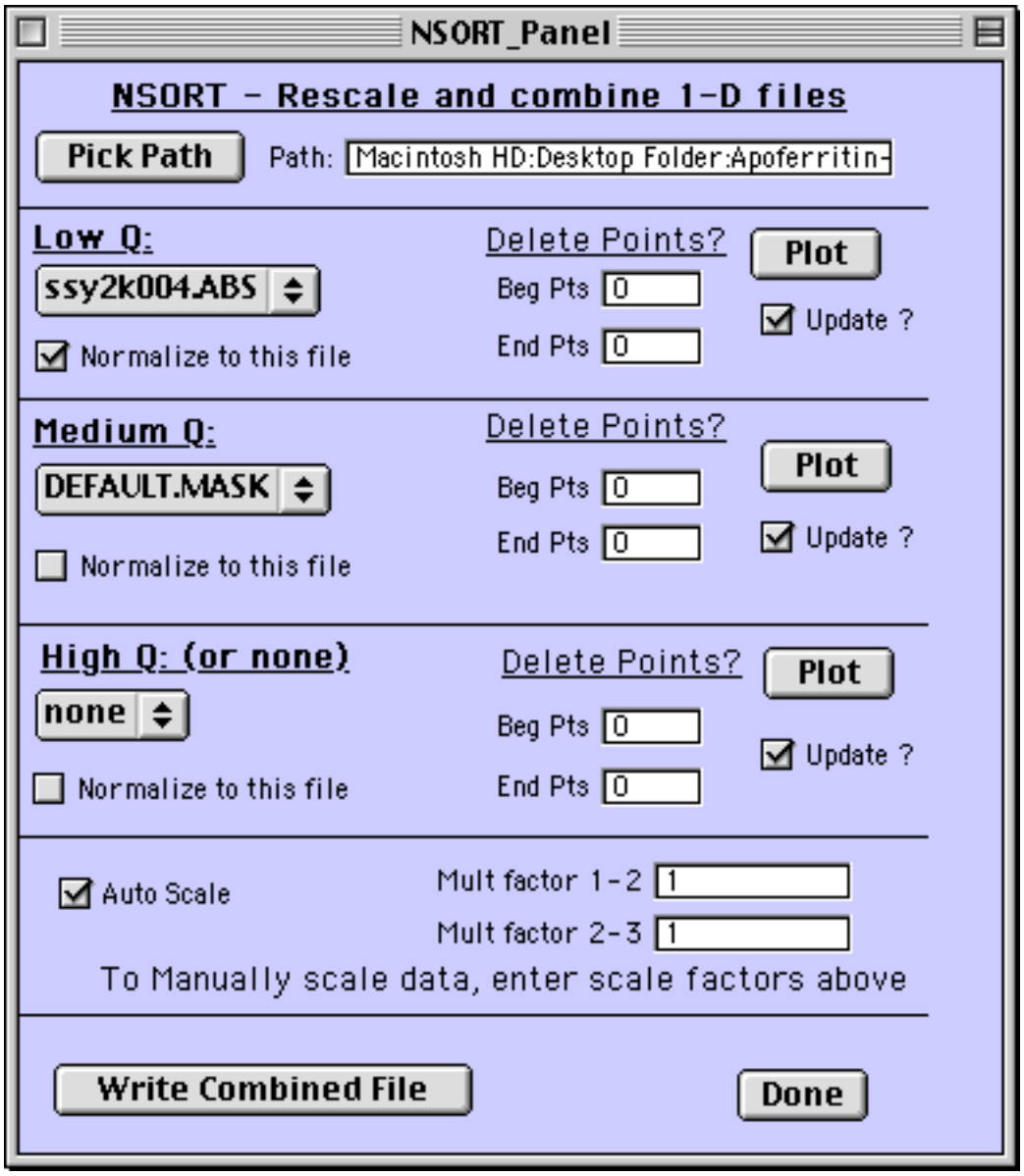
• If you see a message that "This file has already been loaded..." then you will need to "Append Traces to Graph..." from the Graph menu. From the lists, select the y-data (the intensity, ends in "i") and the x-data (q-values, ends in "q") and append to the graph.

Sorting and Combining Averaged Datasets

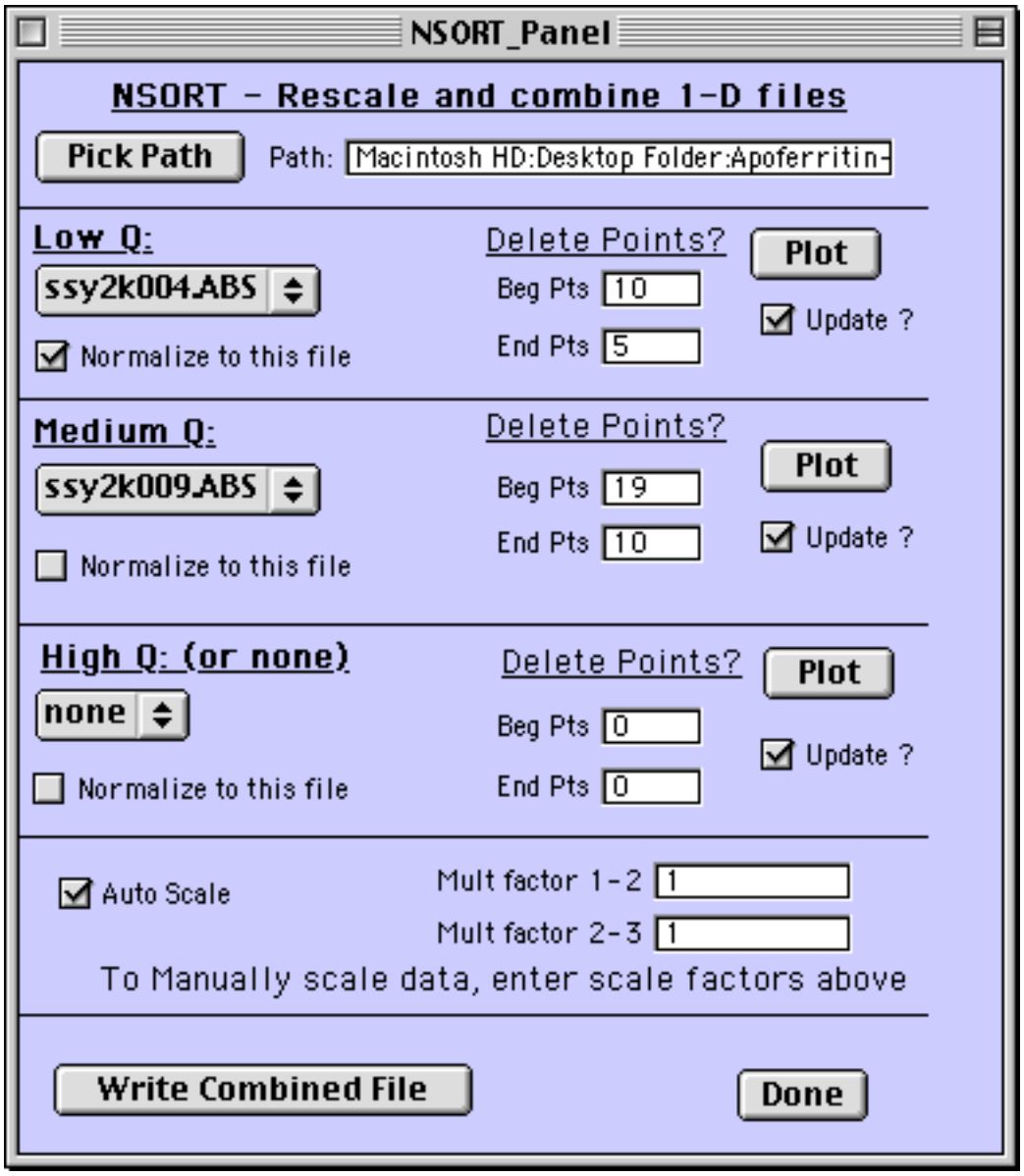
Why: After collecting data at 2 or 3 instrument configurations, it is convenient to combine these data files into a single file, eliminate "bad" data points, and scale the data sets to overlap.

What: Plot the individual data files at the two different q-ranges, trim off the "bad" data points (behind the beamstop and at the corners of the detector), automatically adjust the scaling to get perfect overlap between datasets, and write out the combined data file.

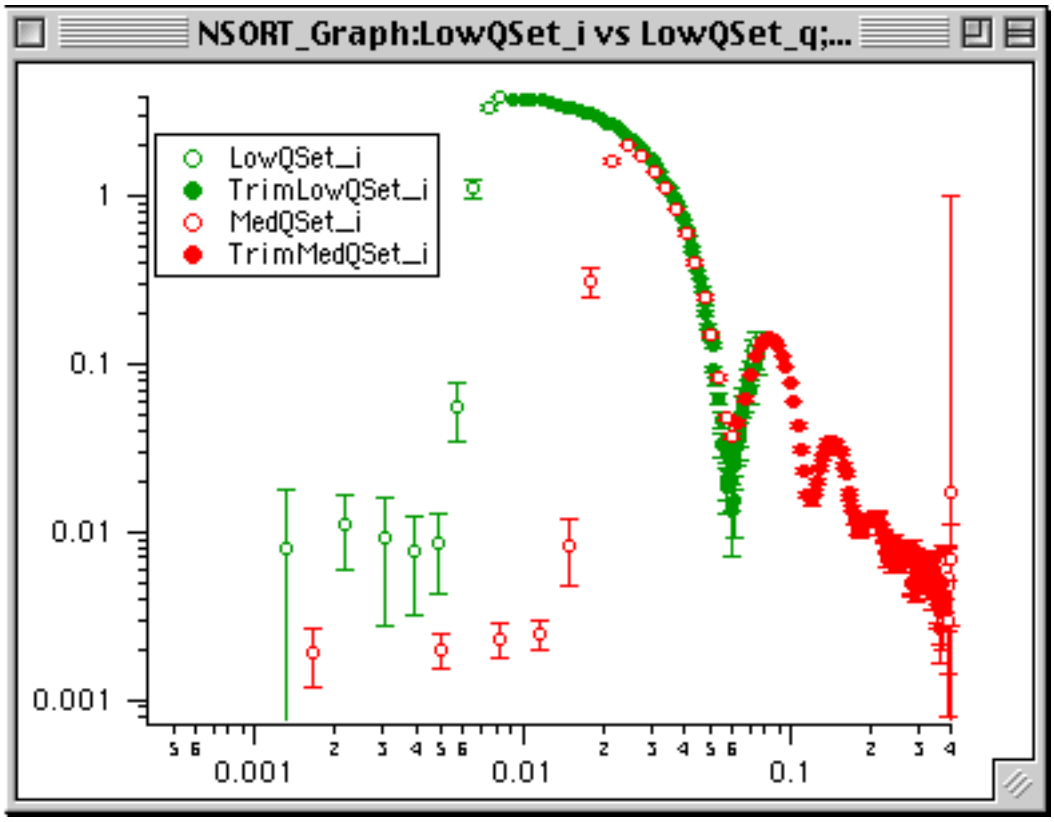
How: Click "NSORT" on the Main Panel. This will display a new panel.



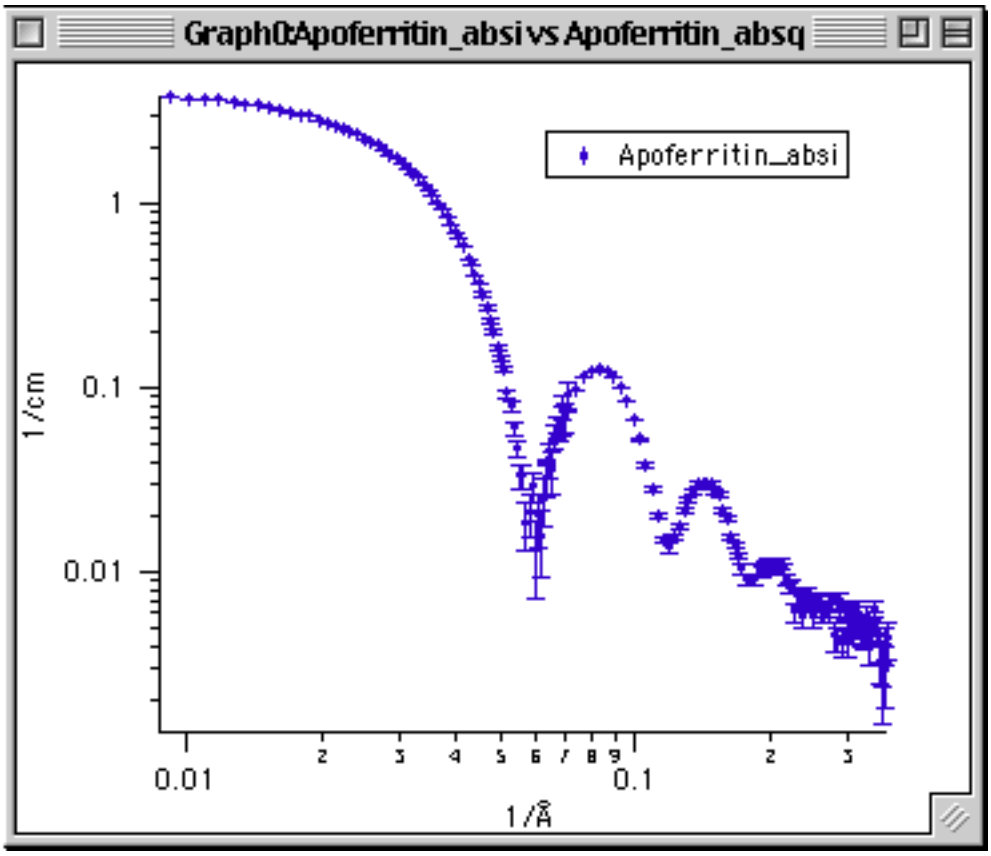
Select the 6-meter data set (the lowest q-values, ssy2k004.abs) as the "Low Q" data file. Plot it, and remove points from the beginning and end of the set that were behind the beamstop or at the edges with large error bars (the omitted points will be displayed as open circles, and are a copy of the original data set). Do the same for the higher q-range (the 1.6-meter set) and the "Medium Q" dataset. If you had a third, still higher q-range, you would plot that set as "High Q", but we have none.



The NSORT graph should look something like this. Be sure "auto scale" is selected for automatic calculation of the overlap constant (or you can enter your own if you wish). Also check the set that you want the combined set to be normalized relative to (you can only choose one). Click "Write Combined File" to create a new file. You will always be prompted for a new name for the combined data set. The header of this file will indicate which files were combined, and the scaling factors used. The scale factor(s) are also copied to the panel. For datasets already on absolute scale, the scaling factor should not be far from unity.



The final, combined and overlapped dataset (I named it Apoferritin.abs), once plotted should look something like this:

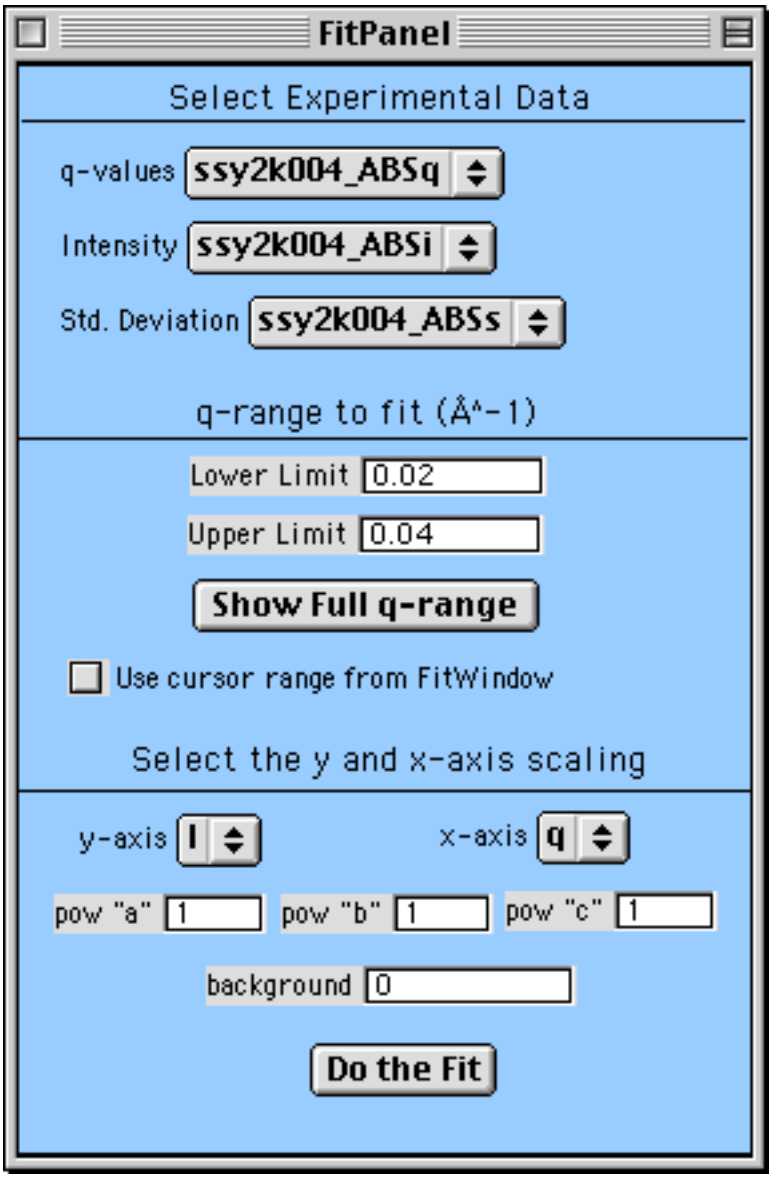


Fitting Lines to Your Data

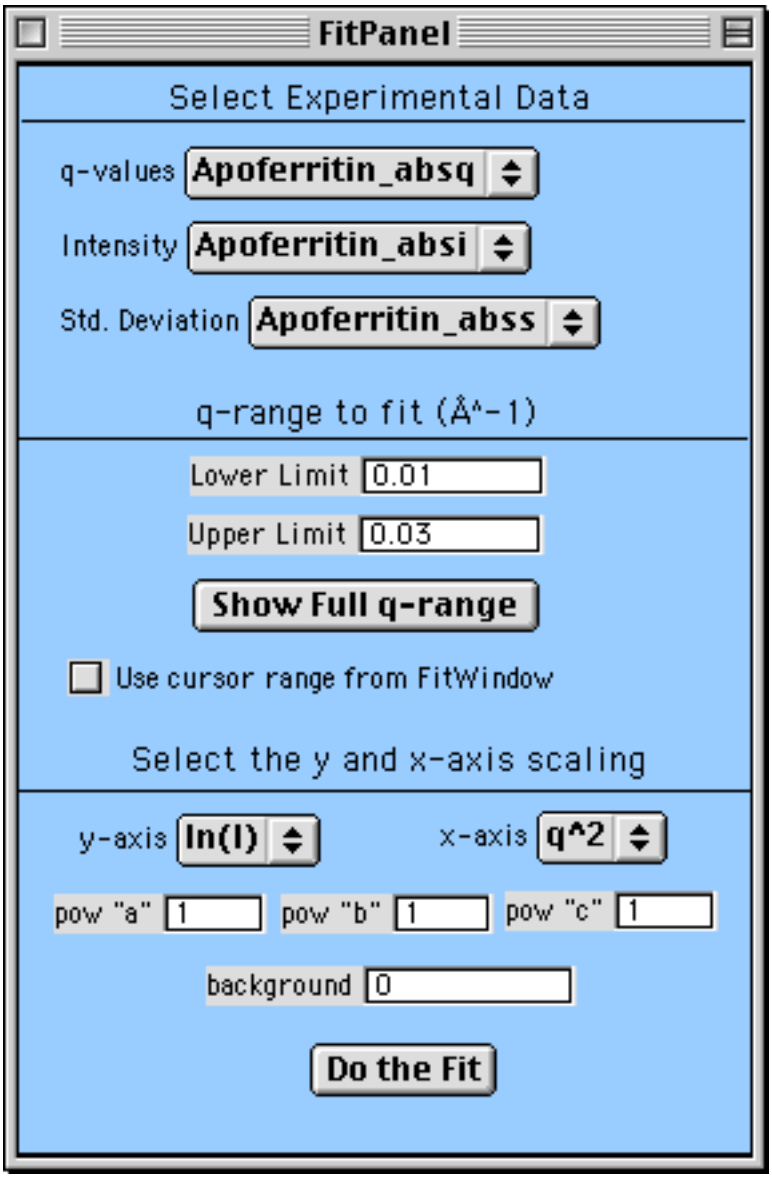
Why: To obtain some quantitative information about your sample.

What: A variety of linearized fits can be performed. Very useful for Guinier fits, Zimm plots, Kratky plots, power laws, etc. Also used to extract absolute scaling parameters from secondary standards (Al-7, water, silica).

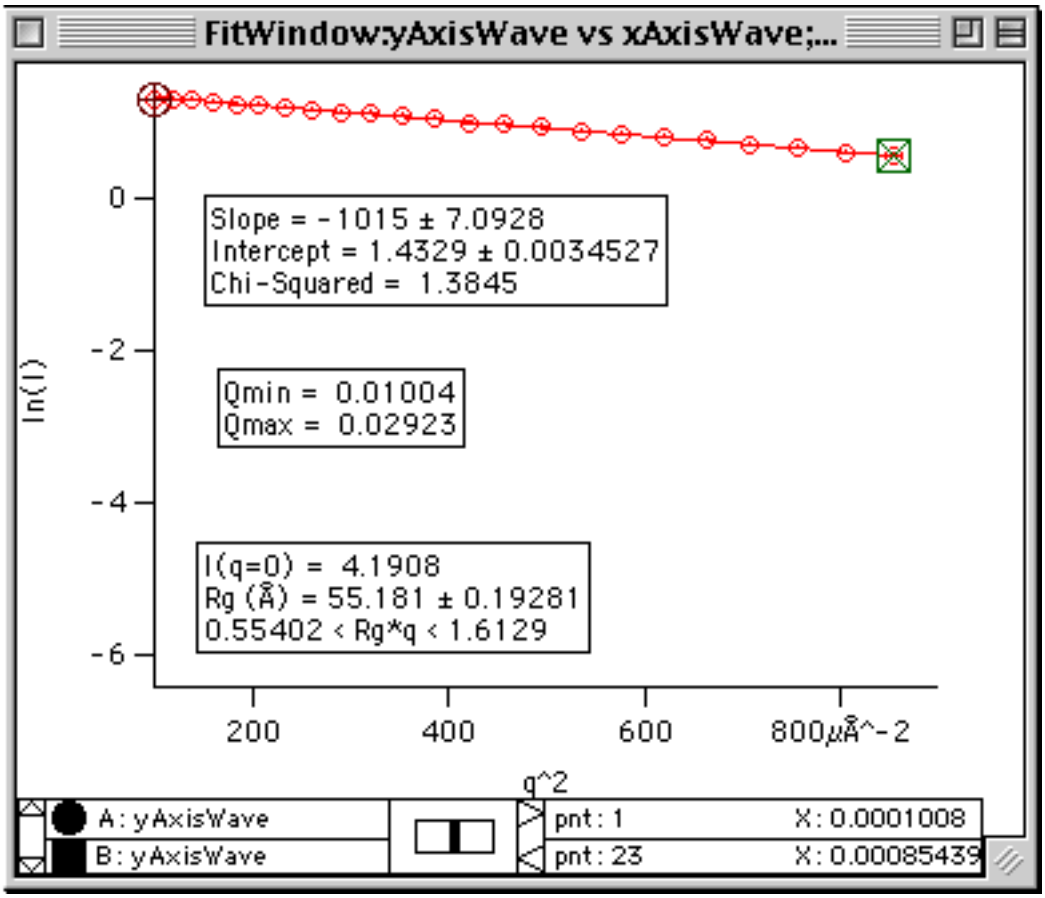
How: The reduced data file Apoferritin.abs is scattering from some sort of protein, and appears to have a Guinier region at low q. Under 1-D operations in the Main Panel, click "Plot" - this will load and plot the averaged apoferritin data set, I (q). If you have already PLOTted the apoferritin data, a dialog will inform you, and you can proceed to the fit. From the Main Panel, click "FIT". The following panel will appear.



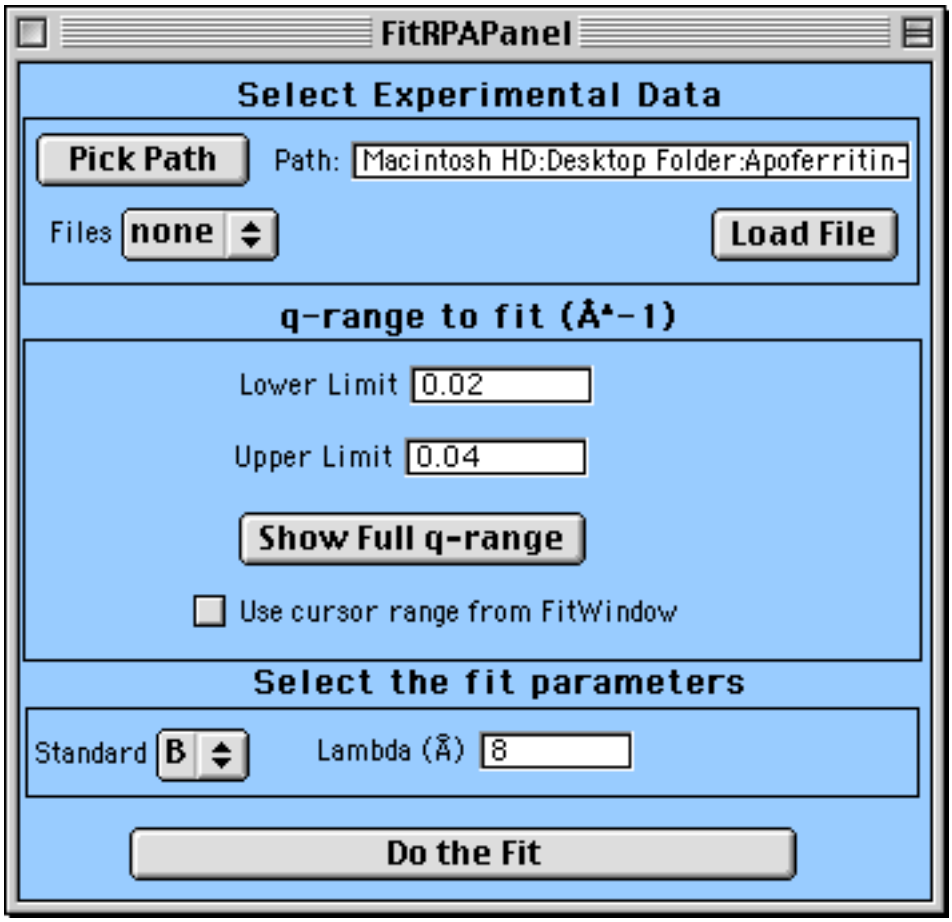
The apoferritin data file that you just plotted should appear in the popup menus for the q, Intensity, and error waves. The name of the **q**-values ends in "abs**q**", the **i**ntensity in "abs**i**", and the **s**tandard deviation of intensity in "abs**s**". Select the appropriate files from the popups. We want to fit this data over the range (0.01 - 0.03) [1/Angstroms]. Enter these values if they are not already there. To fit the data to a Guinier plot for a sphere, select a y-axis scaling of "ln (I)" and an x-axis scaling of "q^2". The powers a, b, and c apply to different axis scalings, and we do not need to subtract any background before doing the fit. Click "Do the Fit", and the data is scaled and fitted, with all the statistics on the graph. One standard deviation is reported along with the radius of gyration and range.



This looks like a good fit, but the fit can be adjusted by either entering new q-values, moving the cursors on the graph to "better" data points, or subtracting a background value before the linearized fit is performed. Clicking "Show Full q-range" does just as stated. The data range that was fitted is marked by the cursors (and is hopefully linear for a Guinier plot).



The secondary polymer standards are fitted with an RPA model (Random Phase Approximation) in order to extract the absolute scaling parameters. This panel "Fit/RPA" behaves much like the FIT panel. The model is specific for the polymer standards, so you need to be sure to chhose the proper standard.

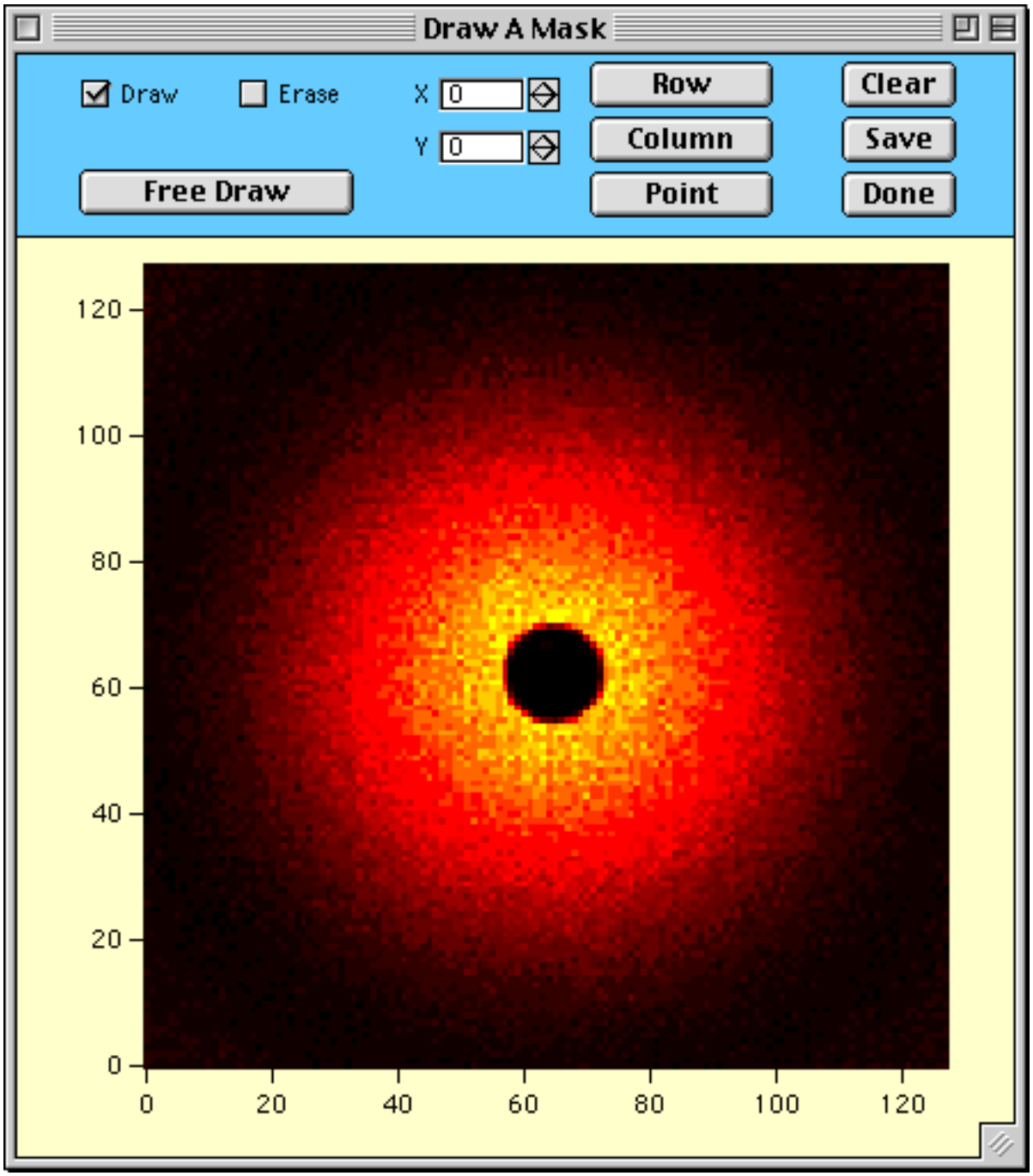


Drawing a Mask

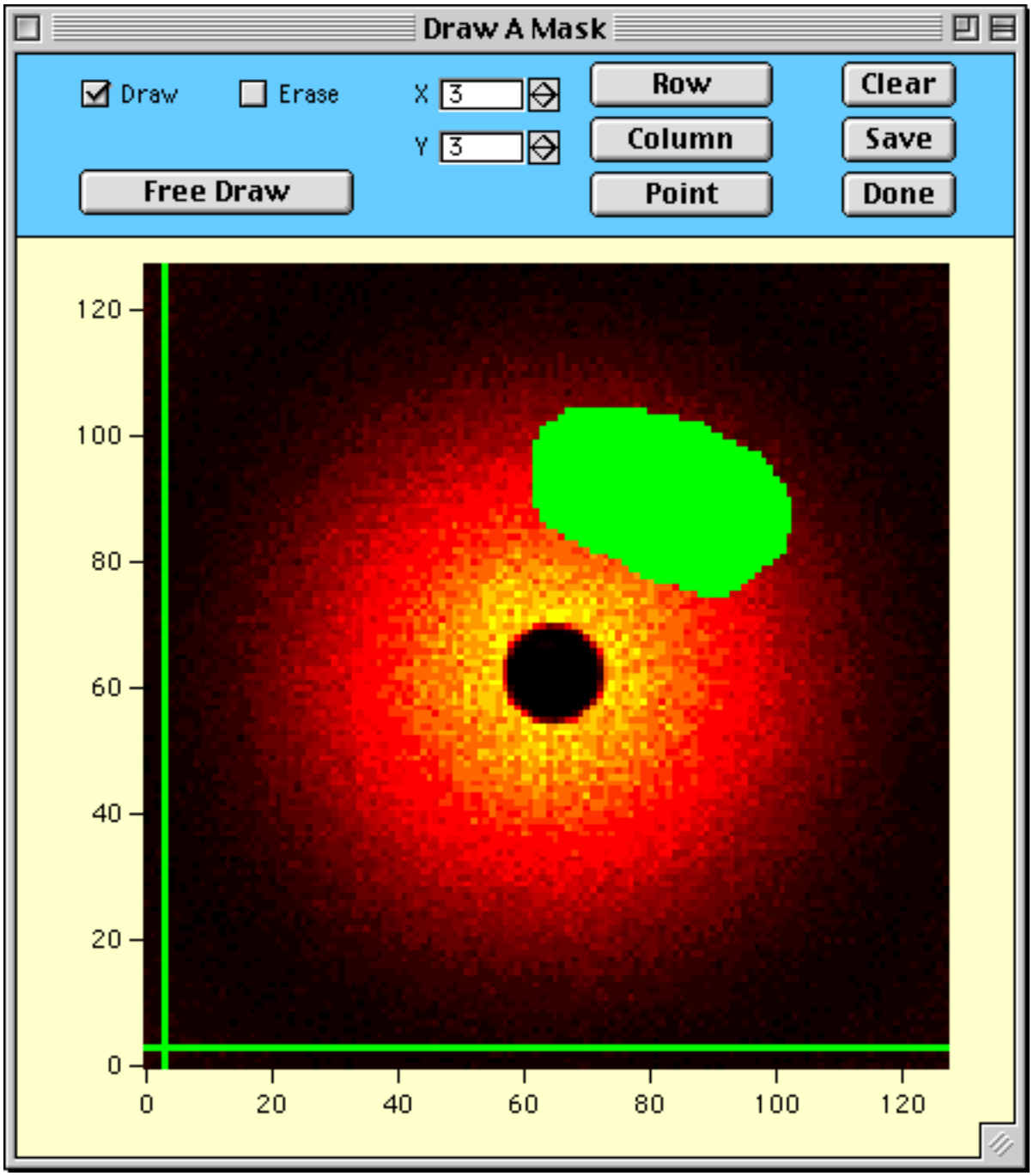
Why: Some pixels on the detector don't yield reliable data, and should be excluded from the averaging.

What: The edges of the detector, typically 2 or 3 channels do not count as reliably as the remainder of the detector, and should not be averaged into 1-D data. This is the usual case, and the "default.mask" should be used. Occasionally a single x or y channel can misbehave. then a custom mask must be drawn, so that the MASKed pixels will be ignored during the averaging step.

How: Display a representative raw data file, then click "Draw Mask" on the main panel. The following window appears. On Windows, you may need to shrink the window size until the white "grid lines" disappear and the image appears continuous.

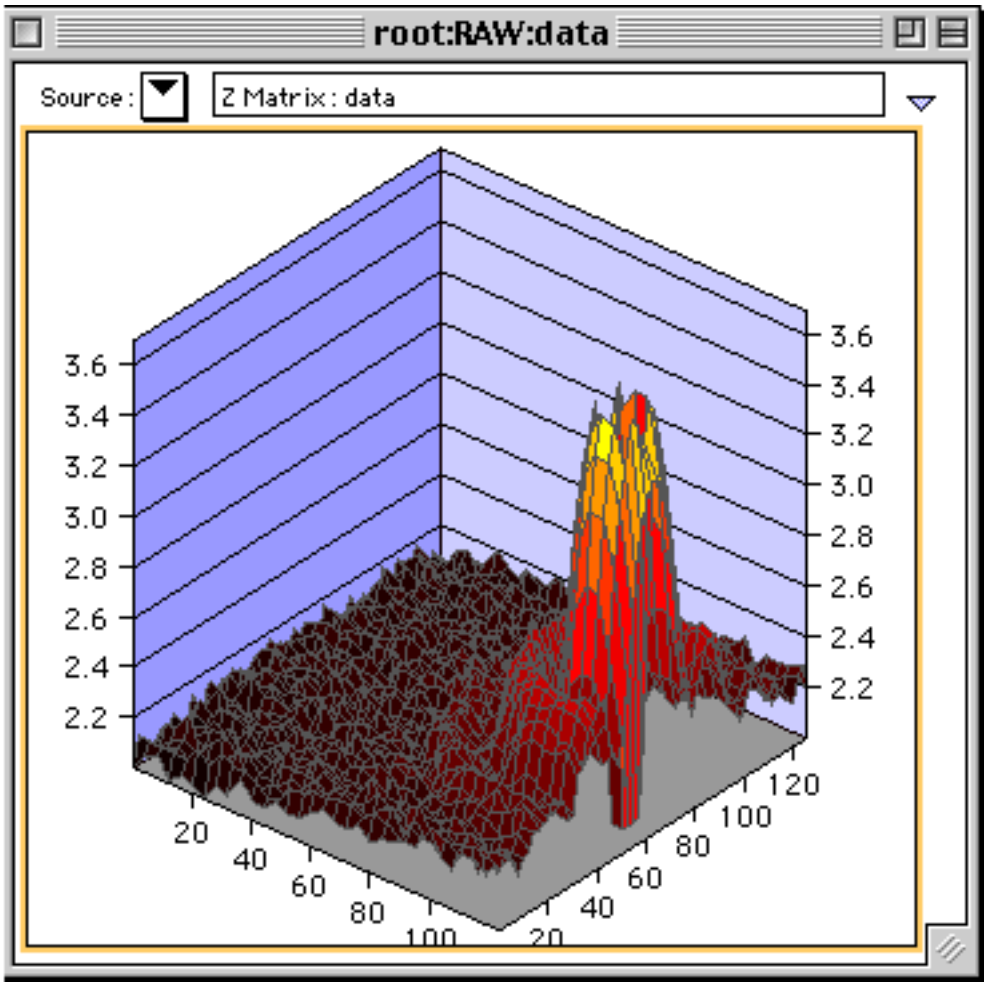


The contol bar allows for draw and erase modes, and allows for rows (y), columns (x), or (x,y) points to be masked. You will always want to mask 2 or 3 channels at each edge of the detector (0,1,2 and 125,126,127) and any other offending regions. The exact pixel locations can be read from the Display window of the same data file. Irregular regions can also be masked by clicking "Free Draw", drawing a region (with the mouse button down), then cicking "Select Points" to fill (or erase) the selected region. Mistakes can be "erased", or "Clear" will start fresh again. Be sure to save your mask before leaving. Once saved, the mask is pre-loaded, and can be immediately viewed on your data by clicking "Show Mask" in the Display window.

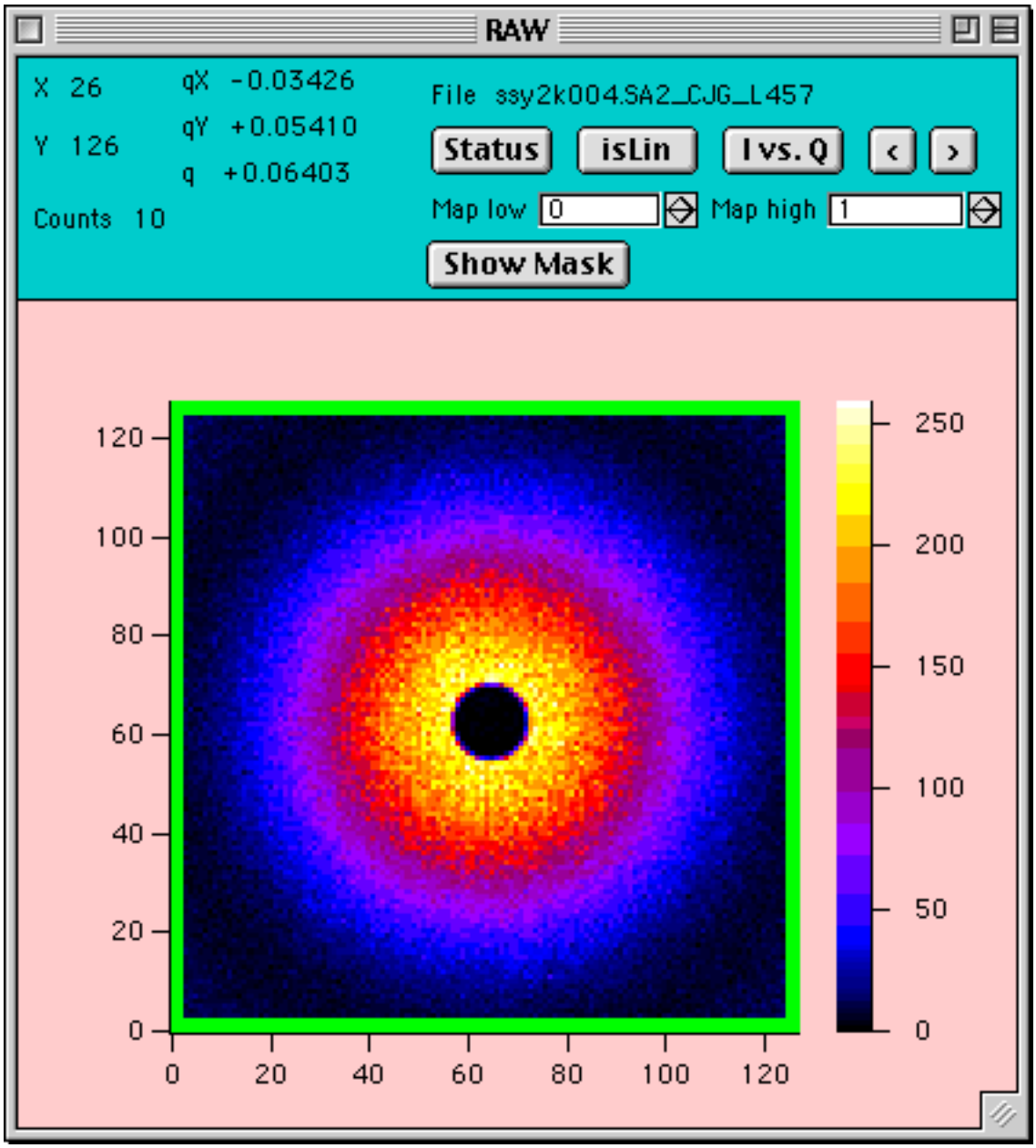


Miscellaneous Operations

• 3-D display of a dataset can be done by clicking "3D Display" on the main panel. Any of the intermediate or raw data files can be displayed, in either log or linear format. To change the scaling, make a 2D display of the same data file, and change its scaling to log or linear as desired - the data in the 3D display will update as well, since it is the same data.



• Mask files can be read in with the "Read Mask" button, since they are not raw SANS data files. A small image of the mask is plotted with the masked region shown in yellow. This mask can be overlayed on the current dataset by using the "Show Mask" button on the display window. Clicking again will toggle the mask off. The scattering data is unaffected by this operation.



• Intermediate 2-D data files (EMPty cell files, BackGrounD, etc.) can be displayed by clicking "Display" on the main panel, under Intermediate 2-D Files. From the popup, choose the desired data type, and continue. If no data of that type exists, you will be informed. Note that for anything other than RAW data, the count value displayed for each pixel will not be true neutron counts, but rather a scaled value that does not necessarily have to be an integer.